

FIG. 2

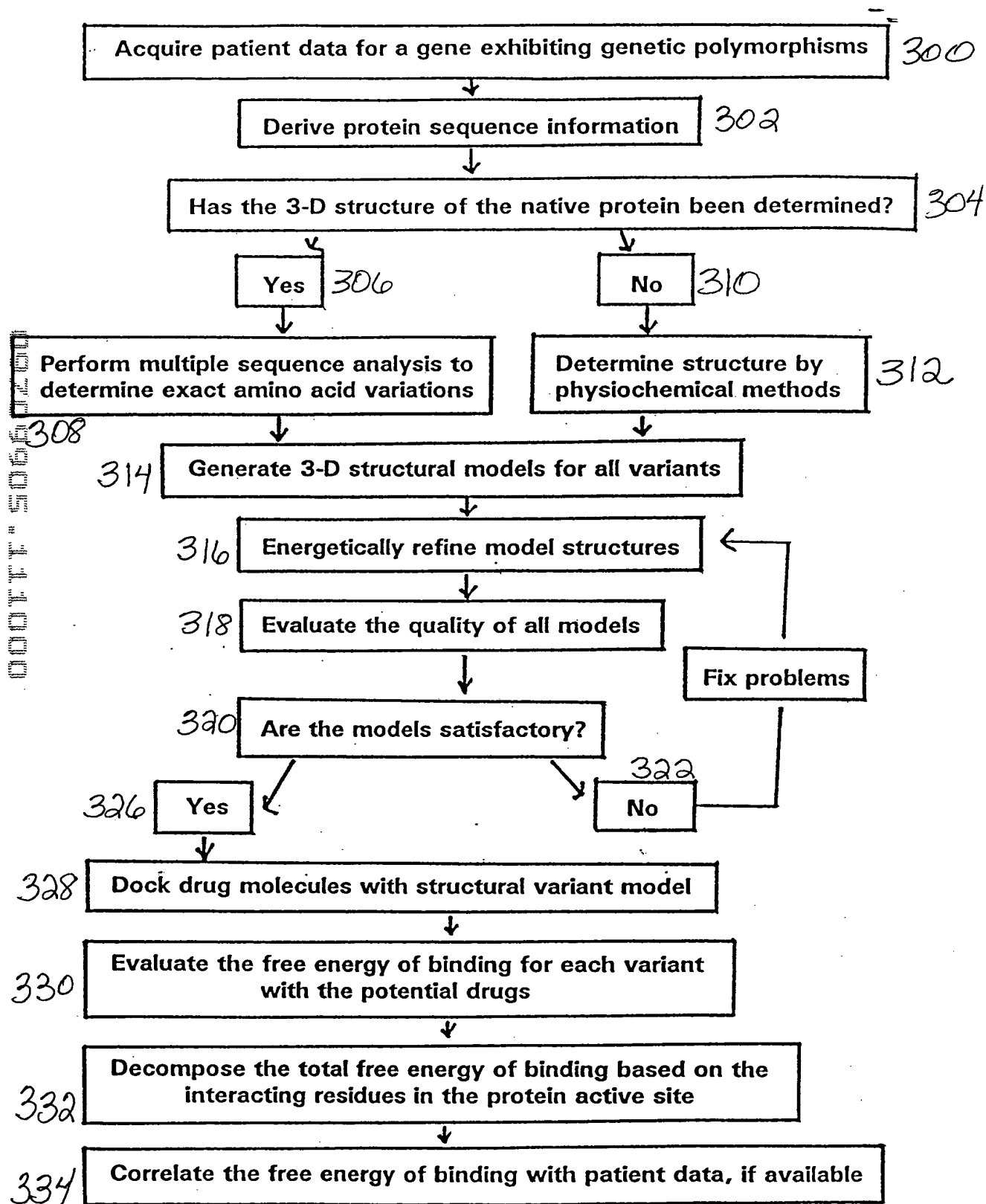
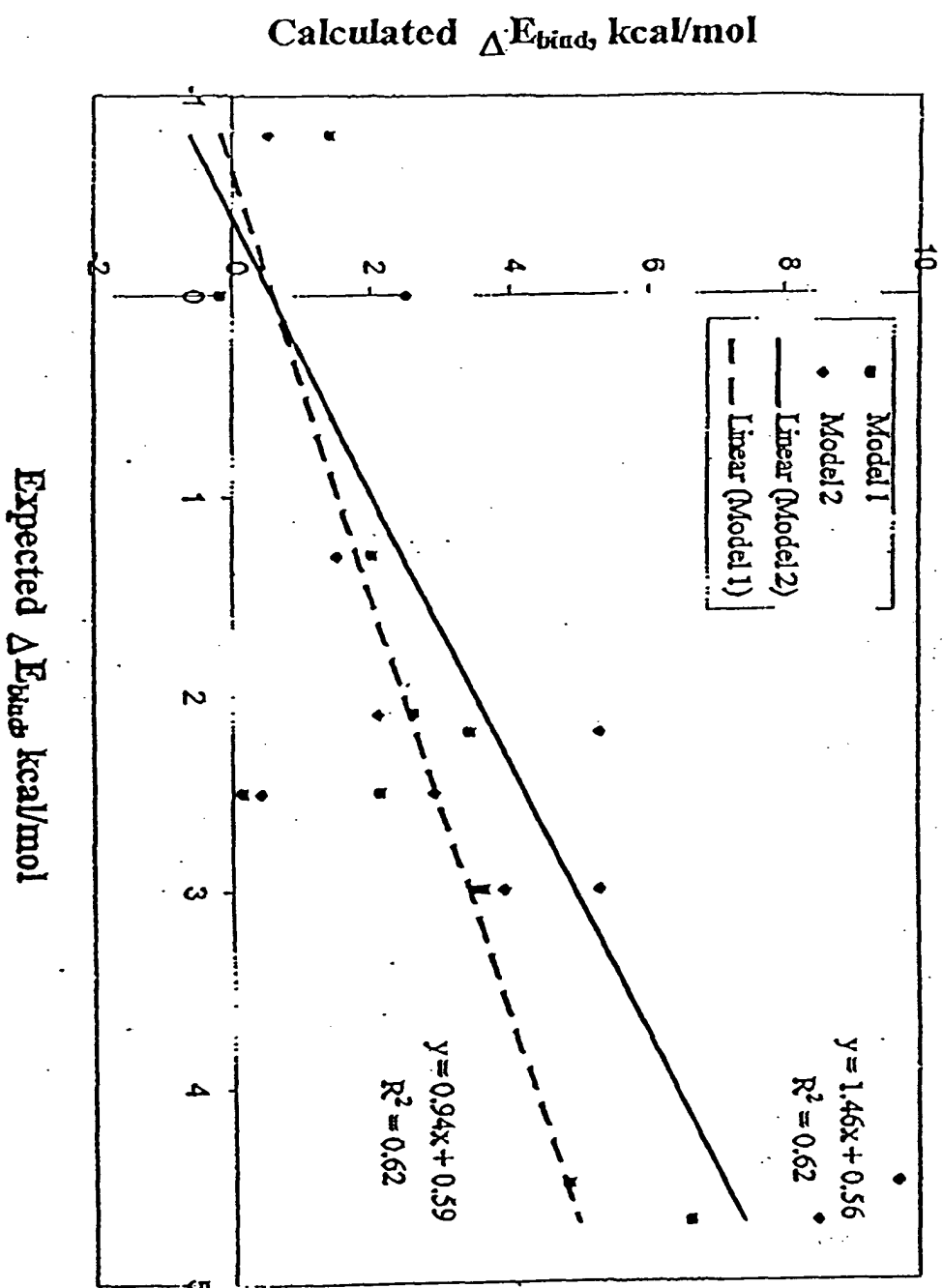


FIG. 3

# Correlation between Experimental and Calculated Changes of Binding Energy upon Ligand Modifications in the Binding Site of NS3



# Comparison of Calculated versus Experimental Binding Free Energy Changes

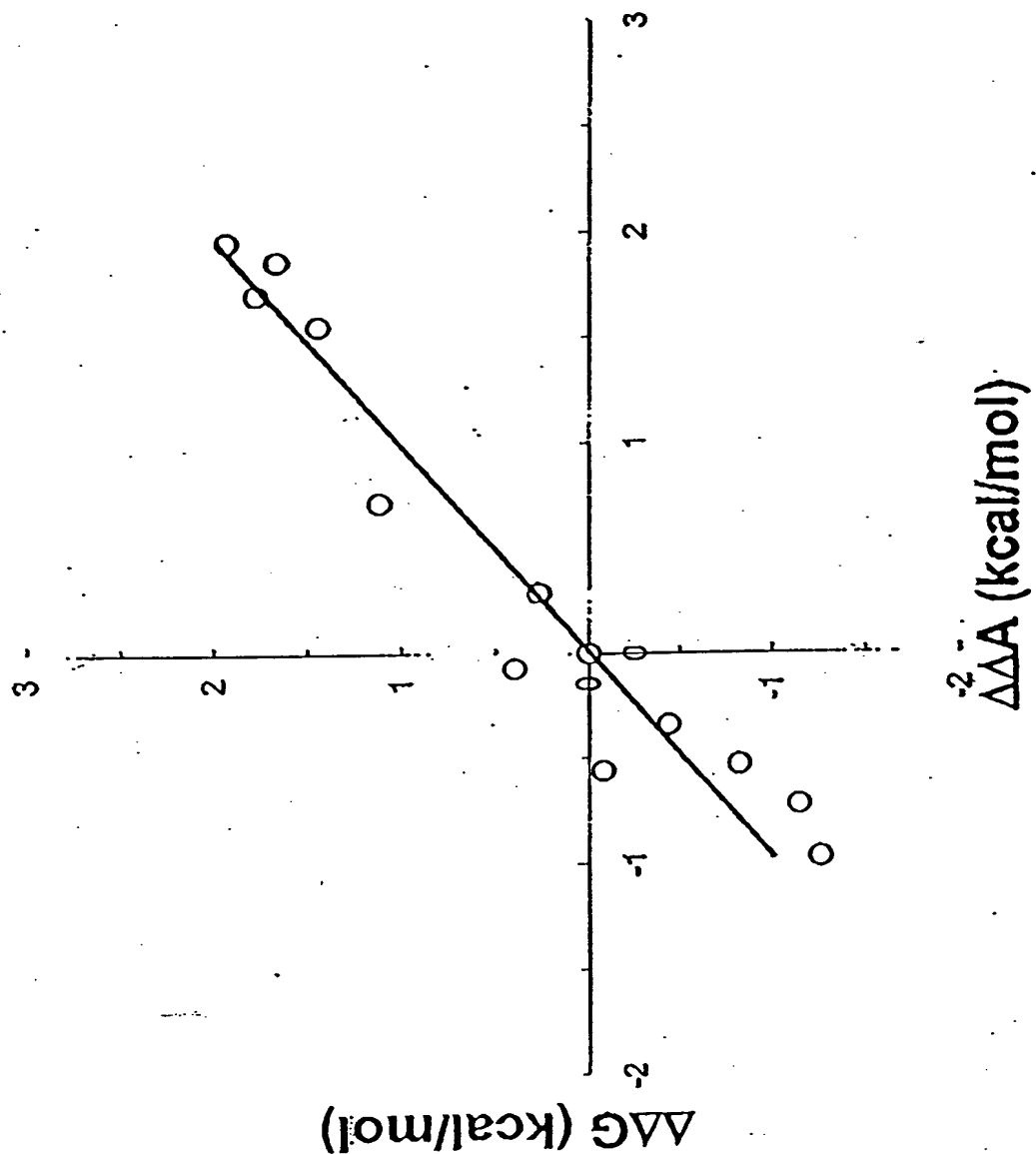
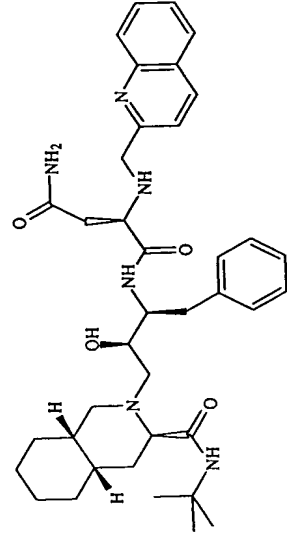
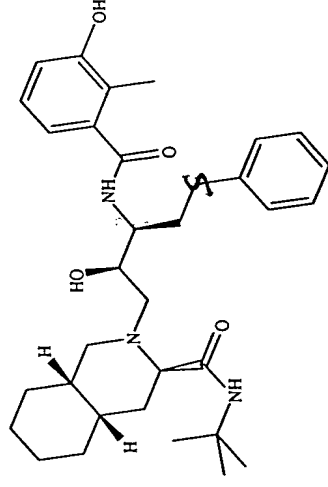


FIG. 5

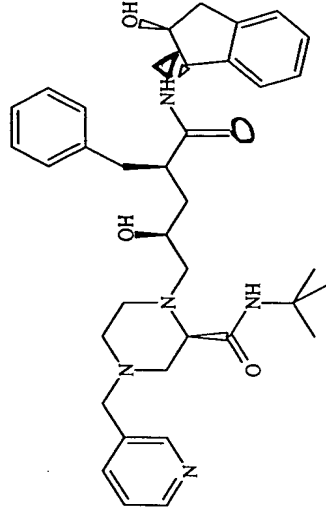
# HIV Protease Inhibitors Approved by FDA



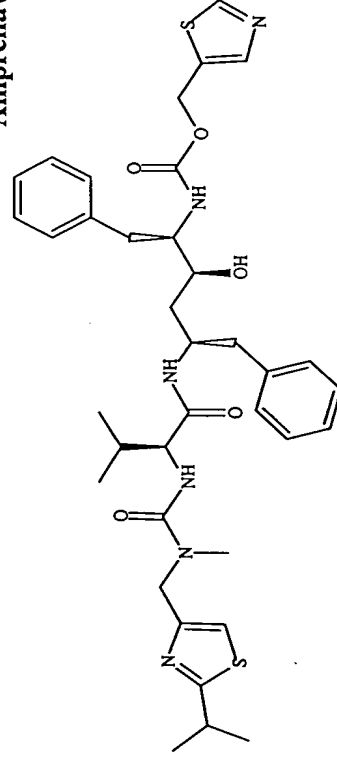
Saquinavir



Nelfinavir



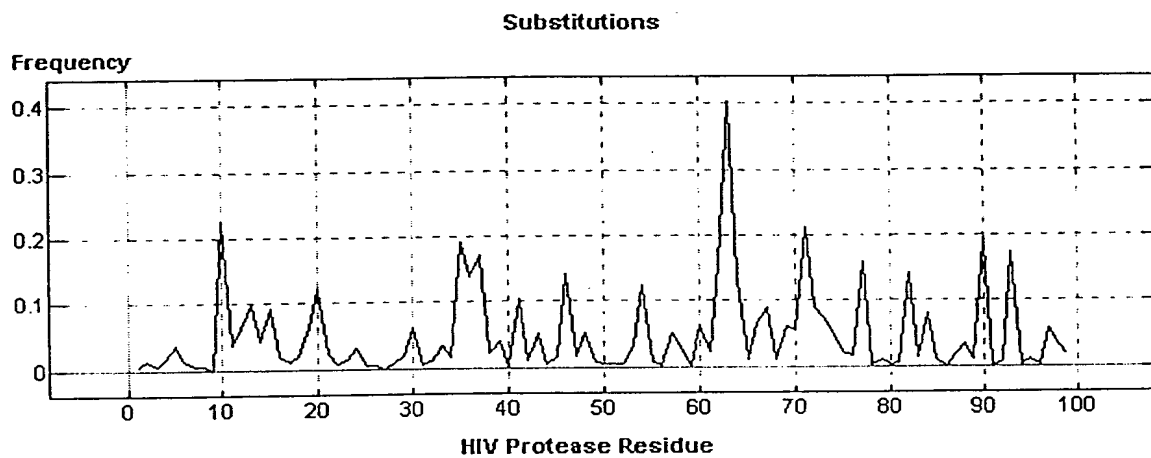
Indinavir



Ritonavir

FIGURE 6

FIGURE 7



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25	28	0	0.0	D	0
26	14	0	3.8	T	0
27	9	0	5.5	G	0
28	16	0	5.8	A	0
29	34	0	8.7	D	0
30	770	7.3	9.2	D	1 N 725
31	15	0	8.9	T	0
32	238	2.2	10.5	V	1 I 221
33	578	5.5	12.4	L	3 VIF 207 189 172
34	88	0	15.1	E	0
35	2790	26.3	18.6	E	1 D 2646
36	2780	26.2	20.2	M	2 IV 2549 129
37	3252	30.7	22.8	N	4 DSET 1253 1129 246 209
38	54	0	22.0	L	0
39	302	2.9	24.9	P	1 S 133
40	19	0	25.5	G	0
41	2249	21.2	26.0	R	1 K 2235
42	21	0	23.5	W	0
43	372	3.5	23.7	K	2 TR 166 144
44	12	0	22.6	P	0
45	208	2	20.0	K	1 R 170
46	2165	20.4	18.8	M	2 TL 1580 560
47	47	0	15.4	I	0
48	445	4.2	14.9	G	1 V 385
49	17	0	12.9	G	0
50	31	0	14.5	I	0
51	24	0	17.6	G	0
52	12	0	18.3	G	0
53	408	3.9	18.1	F	1 L 360

FIGURE 8C

COOTF" 50650460

54	1661	15.7	18.0	I	1	V	1460
55	164	1.5	19.7	K	1	R	149
56	13	0	18.1	V	0		
57	1194	11.3	19.7	R	1	K	1162
58	341	3.2	18.6	Q	1	E	317
59	20	0	19.4	Y	0		
60	992	9.4	19.6	D	1	E	938
61	468	4.4	19.9	Q	1	E	285
62	2711	25.6	18.6	I	1	V	2685
63	8864	83.7	18.5	L	6	PASTQH	7245 380 321 266 226 162
64	2238	21.1	15.8	I	2	VL	1931 223
65	222	2.1	15.6	E	1	D	206
66	194	1.8	12.8	I	0		
67	309	2.9	14.6	C	1	S	143
68	51	0	17.5	G	0		
69	773	7.3	16.1	H	2	QY	376 206
70	478	4.5	17.0	K	1	R	359
71	3664	34.6	15.3	A	3	VTI	2301 1145 190
72	1494	14.1	17.2	I	3	VTL	650 409 126
73	1246	11.8	15.8	G	2	ST	932 185
74	658	6.2	15.4	T	2	SA	433 126
75	73	0	14.1	V	0		
76	59	0	14.6	L	0		
77	3533	33.4	16.1	V	1	I	3513
78	8	0	16.9	G	0		
79	95	0	17.2	P	0		
80	6	0	13.6	T	0		
81	7	0	13.7	P	0		
82	2208	20.8	11.0	V	2	AT	1668 284

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83	44	0	9.7	N	0	
84	1091	10.3	6.3	I	1	V 1073
85	213	2	5.7	I	1	V 198
86	16	0	5.3	G	0	
87	32	0	7.3	R	0	
88	706	6.7	10.4	N	2	DS 543 128
89	240	2.3	10.1	L	1	M 143
90	3429	32.4	8.3	L	1	M 3397
91	28	0	11.4	T	0	
92	227	2.1	13.6	Q	1	K 169
93	3095	29.2	13.1	I	1	L 3041
94	15	0	13.6	G	0	
95	100	0	10.6	C	0	
96	6	0	11.2	T	0	
97	83	0	10.7	L	0	
98	44	0	14.2	N	0	
99	35	0	16.4	F	0	

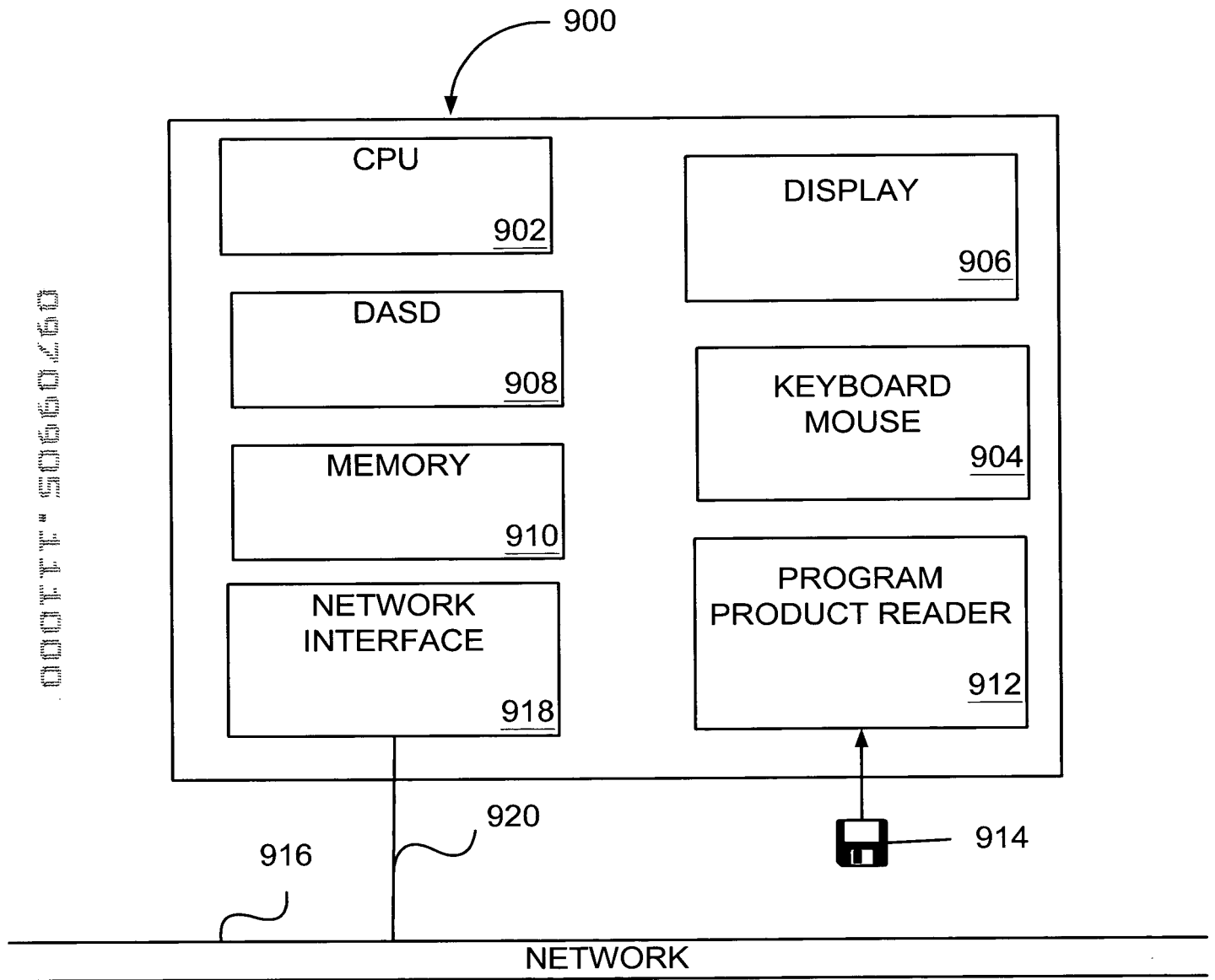


FIG. 9



# Relationships

residue
<b>RESIDUE_ID</b>
VARIANT_ID
CHAIN
RESIDUE_NUMBER
INSERTION_CODE
RESIDUE_CODE

residue_conformation
<b>RESIDUE_CONFORMATION_ID</b>
CONFORMATION_ID
RESIDUE_ID

atom
<b>ATOM_NAME</b>
RESIDUE_CONFORMATION_ID
X_COORDINATE
Y_COORDINATE
Z_COORDINATE

variant
<b>VARIANT_ID</b>
SAMPLE_ID
PROTEIN_ID
NAME
SEQUENCE

conformation
<b>CONFORMATION_ID</b>
MODEL_ID
REFINEMENT_LEVEL

model
<b>MODEL_ID</b>
MODEL_NAME
VARIANT_ID
DRUG_ID

protein
<b>PROTEIN_ID</b>
PROTEIN_NAME
SPECIES
MULTIPLE_DOMAIN
MULTIPLE_CHAIN
WILD_TYPE

resistance_entry
<b>RESISTANCE_ENTRY_ID</b>
PROFILE
PROTEIN_ID
RESIDUAL_NUMBER
AMINO_ACID
WEIGHT
MAXIMUM_WEIGHT

drug
<b>DRUG_ID</b>
PROFILE
SYMBOL
NAME1
NAME2
COMPANY
URL

family
<b>FAMILY_ID</b>
FAMILY_NAME

subfamily
<b>SUBFAMILY_ID</b>
SUBFAMILY_NAME
FAMILY_ID

sample
<b>SAMPLE_ID</b>
SAMPLE_DATE
SEX
AMBIGUITY_NUMBER
DISTANCE
SEQUENCE_LENGTH
SEQUENCE
CLADE
REGION

FIGURE 10

Figure 11A

090903100

ATOM	1	N	PRO	A	1	-3.433	7.956	34.152
ATOM	2	CA	PRO	A	1	-2.653	6.918	34.784
ATOM	3	C	PRO	A	1	-1.242	7.005	34.259
ATOM	4	O	PRO	A	1	-0.950	7.638	33.216
ATOM	5	CB	PRO	A	1	-3.281	5.601	34.262
ATOM	6	CG	PRO	A	1	-4.191	5.995	33.118
ATOM	7	CD	PRO	A	1	-4.547	7.461	33.339
ATOM	8	1H	PRO	A	1	-2.845	8.493	33.547
ATOM	9	2H	PRO	A	1	-3.824	8.552	34.853
ATOM	10	N	GLN	A	2	-0.259	6.464	35.001
ATOM	11	H	GLN	A	2	-0.475	6.057	35.889
ATOM	12	CA	GLN	A	2	1.115	6.443	34.568
ATOM	13	C	GLN	A	2	1.452	4.993	34.301
ATOM	14	O	GLN	A	2	1.379	4.106	35.173
ATOM	15	CB	GLN	A	2	2.070	6.966	35.653
ATOM	16	CG	GLN	A	2	3.549	6.859	35.240
ATOM	17	CD	GLN	A	2	4.490	7.744	36.054
ATOM	18	OE1	GLN	A	2	4.771	8.888	35.719
ATOM	19	NE2	GLN	A	2	4.980	7.190	37.144
ATOM	20	1HE2	GLN	A	2	5.605	7.702	37.734
ATOM	21	2HE2	GLN	A	2	4.731	6.253	37.390
ATOM	22	N	ILE	A	3	1.784	4.644	33.037
ATOM	23	H	ILE	A	3	1.876	5.351	32.336
ATOM	24	CA	ILE	A	3	2.013	3.257	32.665
ATOM	25	C	ILE	A	3	3.505	3.028	32.473
ATOM	26	O	ILE	A	3	4.242	3.777	31.787
ATOM	27	CB	ILE	A	3	1.226	2.944	31.370
ATOM	28	CG1	ILE	A	3	-0.274	3.239	31.603
ATOM	29	CG2	ILE	A	3	1.427	1.480	30.901
ATOM	30	CD1	ILE	A	3	-1.089	3.219	30.322
ATOM	31	N	THR	A	4	4.071	2.032	33.177
ATOM	32	H	THR	A	4	3.525	1.525	33.844
ATOM	33	CA	THR	A	4	5.451	1.661	33.007
ATOM	34	C	THR	A	4	5.515	0.637	31.901
ATOM	35	O	THR	A	4	4.490	0.143	31.397
ATOM	36	CB	THR	A	4	6.051	1.125	34.324
ATOM	37	OG1	THR	A	4	5.224	0.069	34.791
ATOM	38	HG1	THR	A	4	5.589	-0.299	35.646
ATOM	39	CG2	THR	A	4	6.085	2.212	35.431
ATOM	40	N	LEU	A	5	6.677	0.281	31.405
ATOM	41	H	LEU	A	5	7.518	0.530	31.885
ATOM	42	CA	LEU	A	5	6.754	-0.464	30.177
ATOM	43	C	LEU	A	5	7.432	-1.813	30.356
ATOM	44	O	LEU	A	5	7.940	-2.464	29.426
ATOM	45	CB	LEU	A	5	7.459	0.394	29.128
ATOM	46	CG	LEU	A	5	6.668	1.671	28.775
ATOM	47	CD1	LEU	A	5	7.493	2.649	27.939
ATOM	48	CD2	LEU	A	5	5.345	1.307	28.099
ATOM	49	N	TRP	A	6	7.420	-2.351	31.594
ATOM	50	H	TRP	A	6	7.030	-1.833	32.356
ATOM	51	CA	TRP	A	6	7.958	-3.669	31.865
ATOM	52	C	TRP	A	6	7.071	-4.697	31.204
ATOM	53	O	TRP	A	6	7.520	-5.798	30.828
ATOM	54	CB	TRP	A	6	8.099	-3.913	33.367
ATOM	55	CG	TRP	A	6	9.041	-2.974	34.070



# CONFIDENTIAL

ATOM	112	CA	VAL	A	11	-5.506	-1.398	27.835
ATOM	113	C	VAL	A	11	-6.827	-1.857	27.268
ATOM	114	O	VAL	A	11	-6.924	-2.490	26.198
ATOM	115	CB	VAL	A	11	-5.420	0.143	27.897
ATOM	116	CG1	VAL	A	11	-4.117	0.595	28.551
ATOM	117	CG2	VAL	A	11	-5.549	0.787	26.497
ATOM	118	N	THR	A	12	-7.954	-1.592	27.978
ATOM	119	H	THR	A	12	-7.884	-1.141	28.868
ATOM	120	CA	THR	A	12	-9.301	-1.942	27.496
ATOM	121	C	THR	A	12	-9.889	-0.726	26.795
ATOM	122	O	THR	A	12	-9.856	0.436	27.247
ATOM	123	CB	THR	A	12	-10.225	-2.385	28.659
ATOM	124	OG1	THR	A	12	-9.596	-3.458	29.338
ATOM	125	HG1	THR	A	12	-10.170	-3.766	30.096
ATOM	126	CG2	THR	A	12	-11.579	-2.895	28.156
ATOM	127	N	ILE	A	13	-10.449	-0.932	25.594
ATOM	128	H	ILE	A	13	-10.409	-1.841	25.178
ATOM	129	CA	ILE	A	13	-11.112	0.133	24.882
ATOM	130	C	ILE	A	13	-12.553	-0.292	24.693
ATOM	131	O	ILE	A	13	-12.935	-1.469	24.821
ATOM	132	CB	ILE	A	13	-10.432	0.364	23.511
ATOM	133	CG1	ILE	A	13	-10.466	-0.896	22.628
ATOM	134	CG2	ILE	A	13	-8.986	0.806	23.747
ATOM	135	CD1	ILE	A	13	-9.755	-0.745	21.294
ATOM	136	N	LYS	A	14	-13.470	0.658	24.438
ATOM	137	H	LYS	A	14	-13.209	1.622	24.481
ATOM	138	CA	LYS	A	14	-14.838	0.330	24.100
ATOM	139	C	LYS	A	14	-15.088	0.877	22.719
ATOM	140	O	LYS	A	14	-14.859	2.059	22.375
ATOM	141	CB	LYS	A	14	-15.855	0.916	25.099
ATOM	142	CG	LYS	A	14	-17.325	0.518	24.864
ATOM	143	CD	LYS	A	14	-18.078	0.146	26.166
ATOM	144	CE	LYS	A	14	-18.826	1.342	26.810
ATOM	145	NZ	LYS	A	14	-19.316	0.929	28.173
ATOM	146	1HZ	LYS	A	14	-19.801	1.693	28.599
ATOM	147	3HZ	LYS	A	14	-18.536	0.670	28.743
ATOM	148	2HZ	LYS	A	14	-19.936	0.150	28.082
ATOM	149	N	ILE	A	15	-15.535	0.005	21.798
ATOM	150	H	ILE	A	15	-15.806	-0.916	22.078
ATOM	151	CA	ILE	A	15	-15.642	0.347	20.400
ATOM	152	C	ILE	A	15	-16.894	-0.328	19.887
ATOM	153	O	ILE	A	15	-17.115	-1.542	20.041
ATOM	154	CB	ILE	A	15	-14.382	-0.132	19.639
ATOM	155	CG1	ILE	A	15	-14.478	0.148	18.125
ATOM	156	CG2	ILE	A	15	-14.082	-1.623	19.880
ATOM	157	CD1	ILE	A	15	-14.237	1.603	17.796
ATOM	158	N	GLY	A	16	-17.843	0.435	19.308
ATOM	159	H	GLY	A	16	-17.720	1.426	19.260
ATOM	160	CA	GLY	A	16	-19.053	-0.143	18.745
ATOM	161	C	GLY	A	16	-19.897	-0.817	19.789
ATOM	162	O	GLY	A	16	-20.774	-1.668	19.516
ATOM	163	N	GLY	A	17	-19.712	-0.493	21.088
ATOM	164	H	GLY	A	17	-19.038	0.204	21.334
ATOM	165	CA	GLY	A	17	-20.464	-1.126	22.160
ATOM	166	C	GLY	A	17	-19.718	-2.335	22.653
ATOM	167	O	GLY	A	17	-20.147	-3.098	23.540



Figure 11D

ATOM	168	N	GLN	A	18	-18.507	-2.591	22.121
ATOM	169	H	GLN	A	18	-18.059	-1.900	21.554
ATOM	170	CA	GLN	A	18	-17.806	-3.830	22.326
ATOM	171	C	GLN	A	18	-16.552	-3.549	23.123
ATOM	172	O	GLN	A	18	-15.887	-2.508	22.945
ATOM	173	CB	GLN	A	18	-17.393	-4.294	20.928
ATOM	174	CG	GLN	A	18	-16.911	-5.734	20.788
ATOM	175	CD	GLN	A	18	-18.018	-6.728	20.613
ATOM	176	OE1	GLN	A	18	-19.131	-6.574	21.152
ATOM	177	NE2	GLN	A	18	-17.722	-7.773	19.857
ATOM	178	1HE2	GLN	A	18	-18.404	-8.484	19.689
ATOM	179	2HE2	GLN	A	18	-16.814	-7.860	19.448
ATOM	180	N	LEU	A	19	-16.133	-4.397	24.087
ATOM	181	H	LEU	A	19	-16.682	-5.202	24.312
ATOM	182	CA	LEU	A	19	-14.909	-4.178	24.808
ATOM	183	C	LEU	A	19	-13.799	-4.912	24.090
ATOM	184	O	LEU	A	19	-13.989	-6.018	23.558
ATOM	185	CB	LEU	A	19	-14.982	-4.714	26.254
ATOM	186	CG	LEU	A	19	-15.490	-3.778	27.374
ATOM	187	CD1	LEU	A	19	-16.392	-2.639	26.856
ATOM	188	CD2	LEU	A	19	-16.208	-4.516	28.465
ATOM	189	N	LYS	A	20	-12.603	-4.372	23.978
ATOM	190	H	LYS	A	20	-12.442	-3.448	24.324
ATOM	191	CA	LYS	A	20	-11.507	-5.082	23.365
ATOM	192	C	LYS	A	20	-10.266	-4.618	24.062
ATOM	193	O	LYS	A	20	-10.228	-3.611	24.816
ATOM	194	CB	LYS	A	20	-11.397	-4.798	21.875
ATOM	195	CG	LYS	A	20	-12.558	-5.356	21.100
ATOM	196	CD	LYS	A	20	-12.537	-4.988	19.615
ATOM	197	CE	LYS	A	20	-13.414	-5.958	18.827
ATOM	198	NZ	LYS	A	20	-12.681	-7.208	18.639
ATOM	199	1HZ	LYS	A	20	-13.247	-7.852	18.123
ATOM	200	3HZ	LYS	A	20	-12.458	-7.601	19.531
ATOM	201	2HZ	LYS	A	20	-11.837	-7.027	18.134
ATOM	202	N	GLU	A	21	-9.150	-5.357	23.893
ATOM	203	H	GLU	A	21	-9.185	-6.188	23.338
ATOM	204	CA	GLU	A	21	-7.890	-4.997	24.486
ATOM	205	C	GLU	A	21	-7.001	-4.462	23.390
ATOM	206	O	GLU	A	21	-6.970	-4.992	22.258
ATOM	207	CB	GLU	A	21	-7.268	-6.260	25.051
ATOM	208	CG	GLU	A	21	-5.835	-6.140	25.480
ATOM	209	CD	GLU	A	21	-5.405	-7.352	26.275
ATOM	210	OE1	GLU	A	21	-5.624	-7.343	27.508
ATOM	211	OE2	GLU	A	21	-4.852	-8.309	25.684
ATOM	212	N	ALA	A	22	-6.239	-3.369	23.595
ATOM	213	H	ALA	A	22	-6.223	-2.938	24.497
ATOM	214	CA	ALA	A	22	-5.419	-2.781	22.520
ATOM	215	C	ALA	A	22	-4.138	-2.255	23.114
ATOM	216	O	ALA	A	22	-3.985	-1.914	24.314
ATOM	217	CB	ALA	A	22	-6.134	-1.657	21.821
ATOM	218	N	LEU	A	23	-3.121	-2.091	22.240
ATOM	219	H	LEU	A	23	-3.279	-2.236	21.263
ATOM	220	CA	LEU	A	23	-1.797	-1.712	22.640
ATOM	221	C	LEU	A	23	-1.660	-0.230	22.443
ATOM	222	O	LEU	A	23	-2.020	0.349	21.402
ATOM	223	CB	LEU	A	23	-0.814	-2.486	21.732

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Figure 11E

ATOM	224	CG	LEU	A	23	0.705	-2.448	21.991
ATOM	225	CD1	LEU	A	23	1.088	-3.400	23.124
ATOM	226	CD2	LEU	A	23	1.462	-2.878	20.708
ATOM	227	N	LEU	A	24	-1.192	0.530	23.463
ATOM	228	H	LEU	A	24	-1.015	0.110	24.353
ATOM	229	CA	LEU	A	24	-0.935	1.952	23.305
ATOM	230	C	LEU	A	24	0.403	2.089	22.609
ATOM	231	O	LEU	A	24	1.471	1.717	23.130
ATOM	232	CB	LEU	A	24	-0.921	2.609	24.681
ATOM	233	CG	LEU	A	24	-2.220	2.492	25.477
ATOM	234	CD1	LEU	A	24	-2.063	3.291	26.772
ATOM	235	CD2	LEU	A	24	-3.419	3.000	24.691
ATOM	236	N	ASP	A	25	0.454	2.590	21.397
ATOM	237	H	ASP	A	25	-0.334	3.085	21.032
ATOM	238	CA	ASP	A	25	1.642	2.423	20.605
ATOM	239	C	ASP	A	25	2.130	3.750	20.059
ATOM	240	O	ASP	A	25	1.568	4.320	19.110
ATOM	241	CB	ASP	A	25	1.263	1.435	19.486
ATOM	242	CG	ASP	A	25	2.428	1.051	18.561
ATOM	243	OD1	ASP	A	25	3.546	1.540	18.729
ATOM	244	OD2	ASP	A	25	2.164	0.241	17.658
ATOM	245	N	THR	A	26	3.203	4.337	20.605
ATOM	246	H	THR	A	26	3.694	3.880	21.346
ATOM	247	CA	THR	A	26	3.691	5.652	20.144
ATOM	248	C	THR	A	26	4.397	5.583	18.778
ATOM	249	O	THR	A	26	4.642	6.587	18.079
ATOM	250	CB	THR	A	26	4.596	6.219	21.217
ATOM	251	OG1	THR	A	26	5.716	5.324	21.386
ATOM	252	HG1	THR	A	26	6.332	5.676	22.091
ATOM	253	CG2	THR	A	26	3.878	6.320	22.577
ATOM	254	N	GLY	A	27	4.757	4.377	18.298
ATOM	255	H	GLY	A	27	4.526	3.550	18.811
ATOM	256	CA	GLY	A	27	5.481	4.233	17.040
ATOM	257	C	GLY	A	27	4.520	4.190	15.886
ATOM	258	O	GLY	A	27	4.908	4.242	14.696
ATOM	259	N	ALA	A	28	3.197	4.084	16.117
ATOM	260	H	ALA	A	28	2.856	4.091	17.057
ATOM	261	CA	ALA	A	28	2.213	3.955	15.018
ATOM	262	C	ALA	A	28	1.598	5.299	14.750
ATOM	263	O	ALA	A	28	1.062	5.982	15.650
ATOM	264	CB	ALA	A	28	1.117	2.980	15.390
ATOM	265	N	ASP	A	29	1.503	5.744	13.490
ATOM	266	H	ASP	A	29	1.912	5.216	12.746
ATOM	267	CA	ASP	A	29	0.810	6.984	13.213
ATOM	268	C	ASP	A	29	-0.666	6.724	13.327
ATOM	269	O	ASP	A	29	-1.488	7.637	13.568
ATOM	270	CB	ASP	A	29	1.009	7.433	11.775
ATOM	271	CG	ASP	A	29	2.439	7.882	11.412
ATOM	272	OD1	ASP	A	29	3.360	7.856	12.269
ATOM	273	OD2	ASP	A	29	2.606	8.253	10.252
ATOM	274	N	ASP	A	30	-1.143	5.517	12.990
ATOM	275	H	ASP	A	30	-0.508	4.769	12.800
ATOM	276	CA	ASP	A	30	-2.579	5.245	12.887
ATOM	277	C	ASP	A	30	-3.057	4.208	13.867
ATOM	278	O	ASP	A	30	-2.284	3.483	14.546
ATOM	279	CB	ASP	A	30	-2.896	4.758	11.456

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Figure 11F

ATOM	280	CG	ASP	A	30	-2.495	5.768	10.425
ATOM	281	OD1	ASP	A	30	-3.067	6.871	10.423
ATOM	282	OD2	ASP	A	30	-1.596	5.494	9.618
ATOM	283	N	THR	A	31	-4.393	4.076	14.002
ATOM	284	H	THR	A	31	-5.004	4.700	13.515
ATOM	285	CA	THR	A	31	-5.059	3.062	14.829
ATOM	286	C	THR	A	31	-5.565	1.967	13.913
ATOM	287	O	THR	A	31	-6.223	2.169	12.870
ATOM	288	CB	THR	A	31	-6.212	3.725	15.566
ATOM	289	OG1	THR	A	31	-5.668	4.667	16.474
ATOM	290	HG1	THR	A	31	-6.403	5.122	16.976
ATOM	291	CG2	THR	A	31	-7.044	2.702	16.389
ATOM	292	N	VAL	A	32	-5.187	0.713	14.235
ATOM	293	H	VAL	A	32	-4.649	0.555	15.063
ATOM	294	CA	VAL	A	32	-5.517	-0.462	13.437
ATOM	295	C	VAL	A	32	-6.092	-1.506	14.365
ATOM	296	O	VAL	A	32	-5.502	-1.957	15.365
ATOM	297	CB	VAL	A	32	-4.260	-1.064	12.757
ATOM	298	CG1	VAL	A	32	-4.667	-2.136	11.735
ATOM	299	CG2	VAL	A	32	-3.422	0.017	12.032
ATOM	300	N	LEU	A	33	-7.352	-1.923	14.119
ATOM	301	H	LEU	A	33	-7.867	-1.523	13.361
ATOM	302	CA	LEU	A	33	-7.982	-2.940	14.929
ATOM	303	C	LEU	A	33	-8.174	-4.203	14.107
ATOM	304	O	LEU	A	33	-8.268	-4.247	12.853
ATOM	305	CB	LEU	A	33	-9.336	-2.477	15.408
ATOM	306	CG	LEU	A	33	-9.292	-1.149	16.127
ATOM	307	CD1	LEU	A	33	-10.710	-0.747	16.485
ATOM	308	CD2	LEU	A	33	-8.348	-1.139	17.347
ATOM	309	N	GLU	A	34	-8.296	-5.319	14.782
ATOM	310	H	GLU	A	34	-8.244	-5.302	15.780
ATOM	311	CA	GLU	A	34	-8.503	-6.551	14.086
ATOM	312	C	GLU	A	34	-9.909	-6.549	13.510
ATOM	313	O	GLU	A	34	-10.808	-5.717	13.795
ATOM	314	CB	GLU	A	34	-8.265	-7.750	15.010
ATOM	315	CG	GLU	A	34	-9.259	-7.791	16.165
ATOM	316	CD	GLU	A	34	-8.763	-8.552	17.404
ATOM	317	OE1	GLU	A	34	-7.670	-9.193	17.368
ATOM	318	OE2	GLU	A	34	-9.482	-8.497	18.407
ATOM	319	N	GLU	A	35	-10.152	-7.480	12.568
ATOM	320	H	GLU	A	35	-9.485	-8.208	12.407
ATOM	321	CA	GLU	A	35	-11.352	-7.466	11.773
ATOM	322	C	GLU	A	35	-12.631	-7.520	12.571
ATOM	323	O	GLU	A	35	-12.814	-8.294	13.528
ATOM	324	CB	GLU	A	35	-11.237	-8.536	10.707
ATOM	325	CG	GLU	A	35	-9.945	-8.280	9.907
ATOM	326	CD	GLU	A	35	-9.872	-8.872	8.486
ATOM	327	OE1	GLU	A	35	-10.612	-8.401	7.603
ATOM	328	OE2	GLU	A	35	-9.024	-9.776	8.261
ATOM	329	N	MET	A	36	-13.580	-6.598	12.278
ATOM	330	H	MET	A	36	-13.439	-5.967	11.515
ATOM	331	CA	MET	A	36	-14.819	-6.495	13.052
ATOM	332	C	MET	A	36	-15.826	-5.635	12.271
ATOM	333	O	MET	A	36	-15.514	-4.828	11.371
ATOM	334	CB	MET	A	36	-14.593	-5.845	14.428
ATOM	335	CG	MET	A	36	-14.279	-4.353	14.417

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Figure 11c

ATOM	336	SD	MET	A	36	-14.251	-3.718	16.099
ATOM	337	CE	MET	A	36	-12.487	-3.846	16.409
ATOM	338	N	SER	A	37	-17.130	-5.776	12.590
ATOM	339	H	SER	A	37	-17.399	-6.431	13.296
ATOM	340	CA	SER	A	37	-18.155	-5.005	11.940
ATOM	341	C	SER	A	37	-18.286	-3.693	12.657
ATOM	342	O	SER	A	37	-18.593	-3.624	13.865
ATOM	343	CB	SER	A	37	-19.506	-5.688	12.032
ATOM	344	OG	SER	A	37	-19.455	-7.054	11.716
ATOM	345	HG	SER	A	37	-20.367	-7.457	11.791
ATOM	346	N	LEU	A	38	-18.185	-2.569	11.933
ATOM	347	H	LEU	A	38	-17.956	-2.625	10.952
ATOM	348	CA	LEU	A	38	-18.557	-1.247	12.465
ATOM	349	C	LEU	A	38	-19.630	-0.605	11.572
ATOM	350	O	LEU	A	38	-19.706	-0.939	10.391
ATOM	351	CB	LEU	A	38	-17.315	-0.346	12.588
ATOM	352	CG	LEU	A	38	-16.246	-0.818	13.596
ATOM	353	CD1	LEU	A	38	-14.998	0.073	13.489
ATOM	354	CD2	LEU	A	38	-16.756	-0.787	15.046
ATOM	355	N	PRO	A	39	-20.455	0.321	12.108
ATOM	356	CA	PRO	A	39	-21.460	1.053	11.339
ATOM	357	C	PRO	A	39	-20.824	2.176	10.502
ATOM	358	O	PRO	A	39	-19.654	2.519	10.685
ATOM	359	CB	PRO	A	39	-22.430	1.607	12.389
ATOM	360	CG	PRO	A	39	-21.531	1.845	13.600
ATOM	361	CD	PRO	A	39	-20.539	0.686	13.517
ATOM	362	N	GLY	A	40	-21.620	2.749	9.586
ATOM	363	H	GLY	A	40	-22.569	2.417	9.493
ATOM	364	CA	GLY	A	40	-21.203	3.811	8.678
ATOM	365	C	GLY	A	40	-20.836	3.262	7.298
ATOM	366	O	GLY	A	40	-21.405	2.268	6.845
ATOM	367	N	LYS	A	41	-19.895	3.945	6.631
ATOM	368	H	LYS	A	41	-19.496	4.761	7.071
ATOM	369	CA	LYS	A	41	-19.323	3.558	5.343
ATOM	370	C	LYS	A	41	-17.798	3.757	5.371
ATOM	371	O	LYS	A	41	-17.263	4.462	6.229
ATOM	372	CB	LYS	A	41	-20.025	4.352	4.224
ATOM	373	CG	LYS	A	41	-19.703	3.839	2.810
ATOM	374	CD	LYS	A	41	-20.610	4.486	1.757
ATOM	375	CE	LYS	A	41	-20.240	3.964	0.366
ATOM	376	NZ	LYS	A	41	-21.097	4.552	-0.678
ATOM	377	1HZ	LYS	A	41	-20.824	4.189	-1.580
ATOM	378	3HZ	LYS	A	41	-20.993	5.556	-0.673
ATOM	379	2HZ	LYS	A	41	-22.061	4.311	-0.498
ATOM	380	N	TRP	A	42	-17.104	3.091	4.439
ATOM	381	H	TRP	A	42	-17.620	2.548	3.762
ATOM	382	CA	TRP	A	42	-15.654	2.932	4.423
ATOM	383	C	TRP	A	42	-15.105	2.852	2.994
ATOM	384	O	TRP	A	42	-15.845	2.702	2.021
ATOM	385	CB	TRP	A	42	-15.279	1.675	5.236
ATOM	386	CG	TRP	A	42	-16.214	0.514	5.094
ATOM	387	CD1	TRP	A	42	-16.230	-0.402	4.101
ATOM	388	CD2	TRP	A	42	-17.355	0.203	5.942
ATOM	389	NE1	TRP	A	42	-17.297	-1.260	4.281
ATOM	390	HE1	TRP	A	42	-17.504	-2.015	3.644
ATOM	391	CE2	TRP	A	42	-18.045	-0.914	5.389

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Figure 11H

ATOM	392	CE3	TRP	A	42	-17.896	0.792	7.103
ATOM	393	CZ2	TRP	A	42	-19.224	-1.421	5.959
ATOM	394	CZ3	TRP	A	42	-19.077	0.298	7.675
ATOM	395	CH2	TRP	A	42	-19.741	-0.806	7.112
ATOM	396	N	LYS	A	43	-13.771	2.932	2.911
ATOM	397	H	LYS	A	43	-13.260	3.058	3.773
ATOM	398	CA	LYS	A	43	-12.951	2.802	1.713
ATOM	399	C	LYS	A	43	-11.773	1.859	2.012
ATOM	400	O	LYS	A	43	-11.359	1.760	3.166
ATOM	401	CB	LYS	A	43	-12.451	4.193	1.270
ATOM	402	CG	LYS	A	43	-11.724	4.979	2.383
ATOM	403	CD	LYS	A	43	-11.060	6.267	1.873
ATOM	404	CE	LYS	A	43	-9.784	6.001	1.065
ATOM	405	NZ	LYS	A	43	-8.700	5.458	1.903
ATOM	406	1HZ	LYS	A	43	-7.876	5.315	1.338
ATOM	407	3HZ	LYS	A	43	-8.993	4.576	2.300
ATOM	408	2HZ	LYS	A	43	-8.493	6.108	2.647
ATOM	409	N	PRO	A	44	-11.177	1.197	1.004
ATOM	410	CA	PRO	A	44	-9.947	0.435	1.187
ATOM	411	C	PRO	A	44	-8.760	1.392	1.379
ATOM	412	O	PRO	A	44	-8.711	2.434	0.720
ATOM	413	CB	PRO	A	44	-9.808	-0.393	-0.095
ATOM	414	CG	PRO	A	44	-10.501	0.458	-1.159
ATOM	415	CD	PRO	A	44	-11.630	1.132	-0.380
ATOM	416	N	LYS	A	45	-7.790	1.030	2.240
ATOM	417	H	LYS	A	45	-7.912	0.227	2.824
ATOM	418	CA	LYS	A	45	-6.547	1.747	2.314
ATOM	419	C	LYS	A	45	-5.493	0.683	2.507
ATOM	420	O	LYS	A	45	-5.780	-0.470	2.869
ATOM	421	CB	LYS	A	45	-6.594	2.699	3.524
ATOM	422	CG	LYS	A	45	-5.463	3.744	3.609
ATOM	423	CD	LYS	A	45	-5.340	4.289	5.052
ATOM	424	CE	LYS	A	45	-4.262	5.383	5.204
ATOM	425	NZ	LYS	A	45	-2.907	4.911	4.916
ATOM	426	1HZ	LYS	A	45	-2.260	5.664	5.032
ATOM	427	3HZ	LYS	A	45	-2.864	4.577	3.975
ATOM	428	2HZ	LYS	A	45	-2.672	4.169	5.544
ATOM	429	N	MET	A	46	-4.224	0.949	2.193
ATOM	430	H	MET	A	46	-3.998	1.805	1.728
ATOM	431	CA	MET	A	46	-3.157	0.027	2.509
ATOM	432	C	MET	A	46	-2.417	0.701	3.627
ATOM	433	O	MET	A	46	-2.259	1.937	3.634
ATOM	434	CB	MET	A	46	-2.166	-0.088	1.379
ATOM	435	CG	MET	A	46	-2.782	-0.366	0.053
ATOM	436	SD	MET	A	46	-3.076	-2.108	-0.118
ATOM	437	CE	MET	A	46	-1.417	-2.652	-0.186
ATOM	438	N	ILE	A	47	-1.827	-0.016	4.586
ATOM	439	H	ILE	A	47	-2.010	-0.997	4.655
ATOM	440	CA	ILE	A	47	-0.922	0.586	5.539
ATOM	441	C	ILE	A	47	0.233	-0.372	5.654
ATOM	442	O	ILE	A	47	0.135	-1.584	5.356
ATOM	443	CB	ILE	A	47	-1.550	0.836	6.923
ATOM	444	CG1	ILE	A	47	-2.459	-0.301	7.354
ATOM	445	CG2	ILE	A	47	-2.248	2.164	6.995
ATOM	446	CD1	ILE	A	47	-1.724	-1.336	8.111
ATOM	447	N	GLY	A	48	1.420	0.089	6.043



Figure 11J

ATOM	504	CD	LYS	A	55	-8.267	-3.332	1.714
ATOM	505	CE	LYS	A	55	-9.303	-4.392	1.301
ATOM	506	NZ	LYS	A	55	-10.521	-4.453	2.192
ATOM	507	1HZ	LYS	A	55	-11.142	-5.162	1.859
ATOM	508	3HZ	LYS	A	55	-10.987	-3.569	2.180
ATOM	509	2HZ	LYS	A	55	-10.240	-4.669	3.127
ATOM	510	N	VAL	A	56	-6.599	-2.509	4.619
ATOM	511	H	VAL	A	56	-6.337	-1.713	4.073
ATOM	512	CA	VAL	A	56	-7.494	-2.311	5.735
ATOM	513	C	VAL	A	56	-8.711	-1.584	5.236
ATOM	514	O	VAL	A	56	-8.767	-1.029	4.114
ATOM	515	CB	VAL	A	56	-6.759	-1.475	6.812
ATOM	516	CG1	VAL	A	56	-5.569	-2.209	7.385
ATOM	517	CG2	VAL	A	56	-6.287	-0.108	6.268
ATOM	518	N	ARG	A	57	-9.784	-1.539	6.005
ATOM	519	H	ARG	A	57	-9.835	-2.117	6.819
ATOM	520	CA	ARG	A	57	-10.855	-0.648	5.638
ATOM	521	C	ARG	A	57	-10.738	0.534	6.554
ATOM	522	O	ARG	A	57	-10.558	0.449	7.789
ATOM	523	CB	ARG	A	57	-12.219	-1.271	5.835
ATOM	524	CG	ARG	A	57	-12.480	-2.452	4.952
ATOM	525	CD	ARG	A	57	-13.834	-3.051	5.195
ATOM	526	NE	ARG	A	57	-14.122	-4.137	4.270
ATOM	527	HE	ARG	A	57	-13.442	-4.347	3.568
ATOM	528	CZ	ARG	A	57	-15.243	-4.851	4.324
ATOM	529	NH1	ARG	A	57	-16.175	-4.624	5.243
ATOM	530	2HH1	ARG	A	57	-16.044	-3.899	5.920
ATOM	531	1HH1	ARG	A	57	-17.008	-5.178	5.258
ATOM	532	NH2	ARG	A	57	-15.433	-5.822	3.434
ATOM	533	1HH2	ARG	A	57	-16.270	-6.368	3.461
ATOM	534	2HH2	ARG	A	57	-14.738	-6.006	2.738
ATOM	535	N	GLN	A	58	-10.881	1.741	6.036
ATOM	536	H	GLN	A	58	-11.030	1.844	5.053
ATOM	537	CA	GLN	A	58	-10.830	2.922	6.839
ATOM	538	C	GLN	A	58	-12.231	3.342	7.205
ATOM	539	O	GLN	A	58	-13.106	3.608	6.359
ATOM	540	CB	GLN	A	58	-10.208	4.038	6.030
ATOM	541	CG	GLN	A	58	-10.055	5.293	6.817
ATOM	542	CD	GLN	A	58	-9.632	6.411	5.927
ATOM	543	OE1	GLN	A	58	-10.379	7.334	5.662
ATOM	544	NE2	GLN	A	58	-8.412	6.303	5.437
ATOM	545	1HE2	GLN	A	58	-8.047	7.009	4.830
ATOM	546	2HE2	GLN	A	58	-7.843	5.514	5.668
ATOM	547	N	TYR	A	59	-12.527	3.516	8.509
ATOM	548	H	TYR	A	59	-11.877	3.219	9.209
ATOM	549	CA	TYR	A	59	-13.769	4.125	8.933
ATOM	550	C	TYR	A	59	-13.411	5.452	9.565
ATOM	551	O	TYR	A	59	-12.416	5.592	10.310
ATOM	552	CB	TYR	A	59	-14.517	3.252	9.957
ATOM	553	CG	TYR	A	59	-14.287	1.770	9.723
ATOM	554	CD1	TYR	A	59	-13.007	1.269	9.457
ATOM	555	CD2	TYR	A	59	-15.346	0.865	9.766
ATOM	556	CE1	TYR	A	59	-12.797	-0.092	9.240
ATOM	557	CE2	TYR	A	59	-15.148	-0.494	9.551
ATOM	558	CZ	TYR	A	59	-13.873	-0.972	9.287
ATOM	559	OH	TYR	A	59	-13.721	-2.311	9.079

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Figure 1lk

ATOM	560	HH	TYR	A	59	-14.606	-2.771	9.154
ATOM	561	N	ASP	A	60	-14.151	6.542	9.300
ATOM	562	H	ASP	A	60	-14.954	6.464	8.709
ATOM	563	CA	ASP	A	60	-13.822	7.836	9.846
ATOM	564	C	ASP	A	60	-14.782	8.226	10.947
ATOM	565	O	ASP	A	60	-15.941	7.765	11.053
ATOM	566	CB	ASP	A	60	-13.861	8.942	8.769
ATOM	567	CG	ASP	A	60	-12.735	8.830	7.725
ATOM	568	OD1	ASP	A	60	-11.545	8.874	8.075
ATOM	569	OD2	ASP	A	60	-13.060	8.702	6.544
ATOM	570	N	GLN	A	61	-14.339	9.154	11.833
ATOM	571	H	GLN	A	61	-13.385	9.451	11.804
ATOM	572	CA	GLN	A	61	-15.151	9.804	12.885
ATOM	573	C	GLN	A	61	-15.839	8.803	13.802
ATOM	574	O	GLN	A	61	-17.008	8.893	14.229
ATOM	575	CB	GLN	A	61	-16.097	10.908	12.338
ATOM	576	CG	GLN	A	61	-16.239	12.133	13.262
ATOM	577	CD	GLN	A	61	-16.910	13.366	12.629
ATOM	578	OE1	GLN	A	61	-16.509	13.854	11.586
ATOM	579	NE2	GLN	A	61	-17.937	13.887	13.292
ATOM	580	1HE2	GLN	A	61	-18.416	14.689	12.934
ATOM	581	2HE2	GLN	A	61	-18.239	13.482	14.155
ATOM	582	N	ILE	A	62	-15.060	7.760	14.175
ATOM	583	H	ILE	A	62	-14.111	7.714	13.862
ATOM	584	CA	ILE	A	62	-15.557	6.705	15.015
ATOM	585	C	ILE	A	62	-15.251	7.057	16.447
ATOM	586	O	ILE	A	62	-14.198	7.613	16.837
ATOM	587	CB	ILE	A	62	-14.829	5.397	14.653
ATOM	588	CG1	ILE	A	62	-15.253	4.966	13.258
ATOM	589	CG2	ILE	A	62	-15.106	4.271	15.675
ATOM	590	CD1	ILE	A	62	-16.779	4.788	13.116
ATOM	591	N	LEU	A	63	-16.242	6.807	17.320
ATOM	592	H	LEU	A	63	-17.089	6.383	17.000
ATOM	593	CA	LEU	A	63	-16.127	7.131	18.719
ATOM	594	C	LEU	A	63	-15.518	5.942	19.425
ATOM	595	O	LEU	A	63	-15.869	4.753	19.269
ATOM	596	CB	LEU	A	63	-17.512	7.428	19.282
ATOM	597	CG	LEU	A	63	-17.660	7.598	20.813
ATOM	598	CD1	LEU	A	63	-16.711	8.632	21.404
ATOM	599	CD2	LEU	A	63	-19.089	7.963	21.201
ATOM	600	N	ILE	A	64	-14.511	6.211	20.219
ATOM	601	H	ILE	A	64	-14.185	7.153	20.305
ATOM	602	CA	ILE	A	64	-13.862	5.178	20.972
ATOM	603	C	ILE	A	64	-13.529	5.744	22.325
ATOM	604	O	ILE	A	64	-13.396	6.959	22.602
ATOM	605	CB	ILE	A	64	-12.618	4.716	20.231
ATOM	606	CG1	ILE	A	64	-11.925	3.573	20.949
ATOM	607	CG2	ILE	A	64	-11.690	5.865	19.950
ATOM	608	CD1	ILE	A	64	-10.905	2.888	20.062
ATOM	609	N	GLU	A	65	-13.396	4.815	23.294
ATOM	610	H	GLU	A	65	-13.443	3.844	23.059
ATOM	611	CA	GLU	A	65	-13.186	5.174	24.670
ATOM	612	C	GLU	A	65	-12.024	4.360	25.165
ATOM	613	O	GLU	A	65	-11.943	3.112	25.056
ATOM	614	CB	GLU	A	65	-14.459	4.823	25.405
ATOM	615	CG	GLU	A	65	-14.739	5.610	26.646

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ATOM	672	H	ILE	A	72	-12.006	11.517	19.200
ATOM	673	CA	ILE	A	72	-13.376	10.474	17.963
ATOM	674	C	ILE	A	72	-12.480	10.662	16.771
ATOM	675	O	ILE	A	72	-11.858	11.720	16.550
ATOM	676	CB	ILE	A	72	-14.541	11.464	17.882
ATOM	677	CG1	ILE	A	72	-15.306	11.455	19.196
ATOM	678	CG2	ILE	A	72	-15.429	11.203	16.651
ATOM	679	CD1	ILE	A	72	-16.446	12.415	19.176
ATOM	680	N	GLY	A	73	-12.252	9.633	15.958
ATOM	681	H	GLY	A	73	-12.778	8.789	16.067
ATOM	682	CA	GLY	A	73	-11.253	9.755	14.938
ATOM	683	C	GLY	A	73	-11.283	8.554	14.034
ATOM	684	O	GLY	A	73	-12.211	7.706	14.006
ATOM	685	N	THR	A	74	-10.247	8.428	13.182
ATOM	686	H	THR	A	74	-9.471	9.055	13.250
ATOM	687	CA	THR	A	74	-10.201	7.416	12.158
ATOM	688	C	THR	A	74	-9.674	6.134	12.760
ATOM	689	O	THR	A	74	-8.670	6.034	13.497
ATOM	690	CB	THR	A	74	-9.298	7.895	11.048
ATOM	691	OG1	THR	A	74	-9.910	9.019	10.441
ATOM	692	HG1	THR	A	74	-9.335	9.362	9.698
ATOM	693	CG2	THR	A	74	-9.088	6.823	9.946
ATOM	694	N	VAL	A	75	-10.318	5.027	12.327
ATOM	695	H	VAL	A	75	-11.066	5.114	11.669
ATOM	696	CA	VAL	A	75	-9.968	3.717	12.778
ATOM	697	C	VAL	A	75	-9.906	2.843	11.551
ATOM	698	O	VAL	A	75	-10.803	2.807	10.681
ATOM	699	CB	VAL	A	75	-11.044	3.250	13.737
ATOM	700	CG1	VAL	A	75	-11.021	1.721	13.943
ATOM	701	CG2	VAL	A	75	-10.915	4.019	15.034
ATOM	702	N	LEU	A	76	-8.768	2.139	11.366
ATOM	703	H	LEU	A	76	-8.002	2.260	11.998
ATOM	704	CA	LEU	A	76	-8.566	1.183	10.276
ATOM	705	C	LEU	A	76	-8.848	-0.211	10.808
ATOM	706	O	LEU	A	76	-8.514	-0.582	11.958
ATOM	707	CB	LEU	A	76	-7.103	1.270	9.798
ATOM	708	CG	LEU	A	76	-6.608	2.684	9.443
ATOM	709	CD1	LEU	A	76	-5.151	2.645	9.087
ATOM	710	CD2	LEU	A	76	-7.396	3.302	8.296
ATOM	711	N	VAL	A	77	-9.569	-1.062	10.042
ATOM	712	H	VAL	A	77	-9.894	-0.766	9.144
ATOM	713	CA	VAL	A	77	-9.899	-2.428	10.485
ATOM	714	C	VAL	A	77	-9.298	-3.412	9.482
ATOM	715	O	VAL	A	77	-9.450	-3.300	8.253
ATOM	716	CB	VAL	A	77	-11.436	-2.592	10.506
ATOM	717	CG1	VAL	A	77	-11.830	-4.021	10.682
ATOM	718	CG2	VAL	A	77	-12.072	-1.765	11.634
ATOM	719	N	GLY	A	78	-8.560	-4.402	9.928
ATOM	720	H	GLY	A	78	-8.445	-4.530	10.913
ATOM	721	CA	GLY	A	78	-7.930	-5.285	8.987
ATOM	722	C	GLY	A	78	-7.228	-6.380	9.732
ATOM	723	O	GLY	A	78	-7.292	-6.524	10.970
ATOM	724	N	PRO	A	79	-6.512	-7.271	9.003
ATOM	725	CA	PRO	A	79	-5.880	-8.467	9.602
ATOM	726	C	PRO	A	79	-4.599	-8.107	10.340
ATOM	727	O	PRO	A	79	-3.449	-8.489	10.032

Figure 11N

ATOM	728	CB	PRO	A	79	-5.613	-9.379	8.400
ATOM	729	CG	PRO	A	79	-5.529	-8.416	7.210
ATOM	730	CD	PRO	A	79	-6.415	-7.225	7.537
ATOM	731	N	THR	A	80	-4.759	-7.304	11.408
ATOM	732	H	THR	A	80	-5.664	-6.935	11.619
ATOM	733	CA	THR	A	80	-3.658	-6.957	12.263
ATOM	734	C	THR	A	80	-3.490	-8.075	13.308
ATOM	735	O	THR	A	80	-4.447	-8.642	13.857
ATOM	736	CB	THR	A	80	-3.868	-5.572	12.927
ATOM	737	OG1	THR	A	80	-2.770	-5.303	13.787
ATOM	738	HG1	THR	A	80	-2.889	-4.412	14.225
ATOM	739	CG2	THR	A	80	-5.210	-5.464	13.678
ATOM	740	N	PRO	A	81	-2.243	-8.496	13.589
ATOM	741	CA	PRO	A	81	-1.986	-9.476	14.660
ATOM	742	C	PRO	A	81	-2.499	-8.952	16.001
ATOM	743	O	PRO	A	81	-2.944	-9.720	16.866
ATOM	744	CB	PRO	A	81	-0.444	-9.549	14.732
ATOM	745	CG	PRO	A	81	0.069	-8.951	13.429
ATOM	746	CD	PRO	A	81	-1.029	-8.105	12.842
ATOM	747	N	VAL	A	82	-2.474	-7.621	16.276
ATOM	748	H	VAL	A	82	-2.180	-6.975	15.571
ATOM	749	CA	VAL	A	82	-2.869	-7.091	17.591
ATOM	750	C	VAL	A	82	-3.605	-5.761	17.379
ATOM	751	O	VAL	A	82	-3.349	-5.004	16.429
ATOM	752	CB	VAL	A	82	-1.595	-6.858	18.443
ATOM	753	CG1	VAL	A	82	-0.650	-5.824	17.803
ATOM	754	CG2	VAL	A	82	-1.907	-6.418	19.890
ATOM	755	N	ASN	A	83	-4.548	-5.371	18.260
ATOM	756	H	ASN	A	83	-4.810	-5.981	19.007
ATOM	757	CA	ASN	A	83	-5.181	-4.067	18.123
ATOM	758	C	ASN	A	83	-4.195	-3.019	18.565
ATOM	759	O	ASN	A	83	-3.605	-3.064	19.665
ATOM	760	CB	ASN	A	83	-6.436	-3.942	18.982
ATOM	761	CG	ASN	A	83	-7.502	-4.930	18.631
ATOM	762	OD1	ASN	A	83	-7.899	-5.049	17.488
ATOM	763	ND2	ASN	A	83	-7.980	-5.662	19.628
ATOM	764	2HD2	ASN	A	83	-8.695	-6.341	19.459
ATOM	765	1HD2	ASN	A	83	-7.630	-5.541	20.557
ATOM	766	N	ILE	A	84	-4.007	-1.951	17.770
ATOM	767	H	ILE	A	84	-4.583	-1.827	16.962
ATOM	768	CA	ILE	A	84	-2.993	-0.954	18.032
ATOM	769	C	ILE	A	84	-3.679	0.387	18.114
ATOM	770	O	ILE	A	84	-4.460	0.797	17.240
ATOM	771	CB	ILE	A	84	-2.021	-0.922	16.833
ATOM	772	CG1	ILE	A	84	-1.162	-2.150	16.859
ATOM	773	CG2	ILE	A	84	-1.219	0.387	16.747
ATOM	774	CD1	ILE	A	84	-0.375	-2.360	15.579
ATOM	775	N	ILE	A	85	-3.471	1.155	19.203
ATOM	776	H	ILE	A	85	-2.972	0.781	19.985
ATOM	777	CA	ILE	A	85	-3.951	2.518	19.281
ATOM	778	C	ILE	A	85	-2.784	3.425	18.949
ATOM	779	O	ILE	A	85	-1.767	3.515	19.663
ATOM	780	CB	ILE	A	85	-4.522	2.825	20.676
ATOM	781	CG1	ILE	A	85	-5.673	1.865	21.050
ATOM	782	CG2	ILE	A	85	-5.000	4.274	20.716
ATOM	783	CD1	ILE	A	85	-6.828	1.808	20.059

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Figure 11p

ATOM	840	CB	THR	A	91	-2.555	13.543	19.848
ATOM	841	OG1	THR	A	91	-3.459	13.214	18.802
ATOM	842	HG1	THR	A	91	-3.188	13.677	17.958
ATOM	843	CG2	THR	A	91	-1.153	13.122	19.395
ATOM	844	N	GLN	A	92	-5.435	12.704	21.258
ATOM	845	H	GLN	A	92	-5.379	11.892	20.677
ATOM	846	CA	GLN	A	92	-6.763	13.186	21.682
ATOM	847	C	GLN	A	92	-6.942	12.975	23.153
ATOM	848	O	GLN	A	92	-7.554	13.797	23.871
ATOM	849	CB	GLN	A	92	-7.890	12.479	20.964
ATOM	850	CG	GLN	A	92	-7.937	12.862	19.517
ATOM	851	CD	GLN	A	92	-9.251	12.515	18.886
ATOM	852	OE1	GLN	A	92	-10.270	12.424	19.546
ATOM	853	NE2	GLN	A	92	-9.202	12.323	17.588
ATOM	854	1HE2	GLN	A	92	-10.031	12.087	17.080
ATOM	855	2HE2	GLN	A	92	-8.336	12.411	17.097
ATOM	856	N	ILE	A	93	-6.472	11.846	23.721
ATOM	857	H	ILE	A	93	-6.014	11.160	23.155
ATOM	858	CA	ILE	A	93	-6.608	11.578	25.165
ATOM	859	C	ILE	A	93	-5.472	12.189	25.948
ATOM	860	O	ILE	A	93	-5.342	12.031	27.171
ATOM	861	CB	ILE	A	93	-6.820	10.073	25.484
ATOM	862	CG1	ILE	A	93	-5.536	9.221	25.286
ATOM	863	CG2	ILE	A	93	-8.022	9.486	24.735
ATOM	864	CD1	ILE	A	93	-5.754	7.740	25.693
ATOM	865	N	GLY	A	94	-4.594	12.993	25.330
ATOM	866	H	GLY	A	94	-4.617	13.079	24.334
ATOM	867	CA	GLY	A	94	-3.613	13.742	26.063
ATOM	868	C	GLY	A	94	-2.448	12.895	26.512
ATOM	869	O	GLY	A	94	-1.764	13.158	27.519
ATOM	870	N	CYS	A	95	-2.117	11.849	25.797
ATOM	871	H	CYS	A	95	-2.619	11.644	24.957
ATOM	872	CA	CYS	A	95	-1.036	10.994	26.214
ATOM	873	C	CYS	A	95	0.362	11.566	25.925
ATOM	874	O	CYS	A	95	0.588	12.254	24.907
ATOM	875	CB	CYS	A	95	-1.260	9.655	25.550
ATOM	876	SG	CYS	A	95	-0.254	8.307	26.125
ATOM	877	N	THR	A	96	1.346	11.297	26.803
ATOM	878	H	THR	A	96	1.135	10.738	27.618
ATOM	879	CA	THR	A	96	2.728	11.779	26.664
ATOM	880	C	THR	A	96	3.729	10.784	27.264
ATOM	881	O	THR	A	96	3.498	10.249	28.345
ATOM	882	CB	THR	A	96	2.925	13.154	27.346
ATOM	883	OG1	THR	A	96	2.594	13.109	28.721
ATOM	884	HG1	THR	A	96	2.784	13.966	29.109
ATOM	885	CG2	THR	A	96	2.139	14.300	26.698
ATOM	886	N	LEU	A	97	4.882	10.603	26.599
ATOM	887	H	LEU	A	97	5.016	11.071	25.714
ATOM	888	CA	LEU	A	97	6.040	9.910	27.166
ATOM	889	C	LEU	A	97	6.751	10.824	28.175
ATOM	890	O	LEU	A	97	6.705	12.046	28.044
ATOM	891	CB	LEU	A	97	7.013	9.497	26.049
ATOM	892	CG	LEU	A	97	6.452	8.449	25.065
ATOM	893	CD1	LEU	A	97	7.360	8.355	23.828
ATOM	894	CD2	LEU	A	97	6.345	7.065	25.724
ATOM	895	N	ASN	A	98	7.412	10.221	29.175

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Figure 118

ATOM	1007	1HH2	ARG	B	8	5.540	7.860	8.050
ATOM	1008	2HH2	ARG	B	8	4.312	8.281	9.196
ATOM	1009	N	PRO	B	9	7.663	10.381	17.682
ATOM	1010	CA	PRO	B	9	8.666	10.587	18.746
ATOM	1011	C	PRO	B	9	10.065	10.196	18.315
ATOM	1012	O	PRO	B	9	10.678	9.215	18.778
ATOM	1013	CB	PRO	B	9	8.148	9.682	19.878
ATOM	1014	CG	PRO	B	9	7.315	8.607	19.206
ATOM	1015	CD	PRO	B	9	6.708	9.323	18.004
ATOM	1016	N	LEU	B	10	10.685	10.969	17.400
ATOM	1017	H	LEU	B	10	10.201	11.746	16.998
ATOM	1018	CA	LEU	B	10	12.040	10.706	16.978
ATOM	1019	C	LEU	B	10	12.976	11.498	17.850
ATOM	1020	O	LEU	B	10	12.880	12.733	18.018
ATOM	1021	CB	LEU	B	10	12.250	11.170	15.554
ATOM	1022	CG	LEU	B	10	11.427	10.386	14.551
ATOM	1023	CD1	LEU	B	10	11.385	11.175	13.276
ATOM	1024	CD2	LEU	B	10	11.956	8.947	14.355
ATOM	1025	N	VAL	B	11	14.030	10.843	18.384
ATOM	1026	H	VAL	B	11	14.148	9.866	18.206
ATOM	1027	CA	VAL	B	11	15.018	11.517	19.223
ATOM	1028	C	VAL	B	11	16.400	11.111	18.740
ATOM	1029	O	VAL	B	11	16.581	10.201	17.911
ATOM	1030	CB	VAL	B	11	14.857	11.100	20.699
ATOM	1031	CG1	VAL	B	11	13.514	11.586	21.293
ATOM	1032	CG2	VAL	B	11	15.038	9.573	20.903
ATOM	1033	N	THR	B	12	17.485	11.739	19.232
ATOM	1034	H	THR	B	12	17.370	12.507	19.862
ATOM	1035	CA	THR	B	12	18.843	11.325	18.868
ATOM	1036	C	THR	B	12	19.377	10.284	19.837
ATOM	1037	O	THR	B	12	19.237	10.352	21.082
ATOM	1038	CB	THR	B	12	19.830	12.520	18.820
ATOM	1039	OG1	THR	B	12	19.389	13.483	17.876
ATOM	1040	HG1	THR	B	12	20.028	14.252	17.848
ATOM	1041	CG2	THR	B	12	21.234	12.075	18.399
ATOM	1042	N	ILE	B	13	20.044	9.234	19.338
ATOM	1043	H	ILE	B	13	20.135	9.130	18.348
ATOM	1044	CA	ILE	B	13	20.641	8.239	20.176
ATOM	1045	C	ILE	B	13	22.119	8.226	19.855
ATOM	1046	O	ILE	B	13	22.579	8.817	18.865
ATOM	1047	CB	ILE	B	13	19.993	6.870	19.879
ATOM	1048	CG1	ILE	B	13	20.192	6.464	18.415
ATOM	1049	CG2	ILE	B	13	18.482	6.893	20.206
ATOM	1050	CD1	ILE	B	13	19.829	5.035	18.106
ATOM	1051	N	LYS	B	14	22.973	7.618	20.661
ATOM	1052	H	LYS	B	14	22.652	7.243	21.531
ATOM	1053	CA	LYS	B	14	24.364	7.480	20.317
ATOM	1054	C	LYS	B	14	24.680	6.029	20.477
ATOM	1055	O	LYS	B	14	24.353	5.353	21.484
ATOM	1056	CB	LYS	B	14	25.266	8.263	21.242
ATOM	1057	CG	LYS	B	14	24.947	9.729	21.236
ATOM	1058	CD	LYS	B	14	25.664	10.498	22.339
ATOM	1059	CE	LYS	B	14	26.758	11.441	21.807
ATOM	1060	NZ	LYS	B	14	28.026	10.781	21.440
ATOM	1061	1HZ	LYS	B	14	28.674	11.466	21.107
ATOM	1062	3HZ	LYS	B	14	27.855	10.107	20.722

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Figure 11U

ATOM	1119	CA	GLU	B	21	17.735	9.366	15.008
ATOM	1120	C	GLU	B	21	16.937	8.095	15.119
ATOM	1121	O	GLU	B	21	17.117	7.103	14.376
ATOM	1122	CB	GLU	B	21	17.143	10.314	13.983
ATOM	1123	CG	GLU	B	21	15.714	10.706	14.162
ATOM	1124	CD	GLU	B	21	15.304	11.607	13.036
ATOM	1125	OE1	GLU	B	21	14.971	11.051	11.957
ATOM	1126	OE2	GLU	B	21	15.338	12.854	13.174
ATOM	1127	N	ALA	B	22	16.025	7.999	16.072
ATOM	1128	H	ALA	B	22	15.825	8.792	16.648
ATOM	1129	CA	ALA	B	22	15.300	6.783	16.315
ATOM	1130	C	ALA	B	22	13.981	7.132	16.952
ATOM	1131	O	ALA	B	22	13.756	8.153	17.632
ATOM	1132	CB	ALA	B	22	16.095	5.865	17.235
ATOM	1133	N	LEU	B	23	12.994	6.230	16.743
ATOM	1134	H	LEU	B	23	13.195	5.379	16.257
ATOM	1135	CA	LEU	B	23	11.639	6.408	17.180
ATOM	1136	C	LEU	B	23	11.476	5.740	18.534
ATOM	1137	O	LEU	B	23	11.814	4.564	18.746
ATOM	1138	CB	LEU	B	23	10.775	5.665	16.192
ATOM	1139	CG	LEU	B	23	9.267	5.810	16.237
ATOM	1140	CD1	LEU	B	23	8.807	7.142	15.664
ATOM	1141	CD2	LEU	B	23	8.648	4.625	15.482
ATOM	1142	N	LEU	B	24	10.948	6.455	19.553
ATOM	1143	H	LEU	B	24	10.775	7.433	19.435
ATOM	1144	CA	LEU	B	24	10.613	5.838	20.849
ATOM	1145	C	LEU	B	24	9.271	5.160	20.687
ATOM	1146	O	LEU	B	24	8.208	5.764	20.418
ATOM	1147	CB	LEU	B	24	10.564	6.878	21.971
ATOM	1148	CG	LEU	B	24	11.828	7.750	22.075
ATOM	1149	CD1	LEU	B	24	11.580	8.859	23.077
ATOM	1150	CD2	LEU	B	24	13.099	6.955	22.388
ATOM	1151	N	ASP	B	25	9.246	3.822	20.809
ATOM	1152	H	ASP	B	25	10.025	3.347	21.218
ATOM	1153	CA	ASP	B	25	8.122	3.030	20.366
ATOM	1154	C	ASP	B	25	7.637	2.136	21.484
ATOM	1155	O	ASP	B	25	8.189	1.048	21.759
ATOM	1156	CB	ASP	B	25	8.613	2.196	19.189
ATOM	1157	CG	ASP	B	25	7.528	1.421	18.511
ATOM	1158	OD1	ASP	B	25	6.422	1.339	19.058
ATOM	1159	OD2	ASP	B	25	7.800	0.897	17.426
ATOM	1160	N	THR	B	26	6.547	2.465	22.157
ATOM	1161	H	THR	B	26	6.067	3.314	21.938
ATOM	1162	CA	THR	B	26	6.025	1.621	23.212
ATOM	1163	C	THR	B	26	5.347	0.369	22.694
ATOM	1164	O	THR	B	26	4.976	-0.550	23.451
ATOM	1165	CB	THR	B	26	5.027	2.389	24.046
ATOM	1166	OG1	THR	B	26	3.927	2.853	23.239
ATOM	1167	HG1	THR	B	26	3.277	3.359	23.806
ATOM	1168	CG2	THR	B	26	5.703	3.603	24.650
ATOM	1169	N	GLY	B	27	5.090	0.245	21.382
ATOM	1170	H	GLY	B	27	5.341	0.983	20.756
ATOM	1171	CA	GLY	B	27	4.457	-0.938	20.867
ATOM	1172	C	GLY	B	27	5.475	-1.992	20.458
ATOM	1173	O	GLY	B	27	5.121	-3.108	20.055
ATOM	1174	N	ALA	B	28	6.792	-1.717	20.495

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Figure 11v

ATOM	1175	H	ALA	B	28	7.104	-0.832	20.841
ATOM	1176	CA	ALA	B	28	7.800	-2.690	20.037
ATOM	1177	C	ALA	B	28	8.371	-3.444	21.259
ATOM	1178	O	ALA	B	28	8.840	-2.807	22.213
ATOM	1179	CB	ALA	B	28	8.924	-1.936	19.358
ATOM	1180	N	ASP	B	29	8.459	-4.787	21.289
ATOM	1181	H	ASP	B	29	8.082	-5.325	20.535
ATOM	1182	CA	ASP	B	29	9.121	-5.441	22.452
ATOM	1183	C	ASP	B	29	10.608	-5.219	22.404
ATOM	1184	O	ASP	B	29	11.345	-5.264	23.412
ATOM	1185	CB	ASP	B	29	8.965	-6.975	22.447
ATOM	1186	CG	ASP	B	29	7.551	-7.477	22.774
ATOM	1187	OD1	ASP	B	29	6.683	-6.693	23.169
ATOM	1188	OD2	ASP	B	29	7.350	-8.686	22.616
ATOM	1189	N	ASP	B	30	11.164	-5.157	21.171
ATOM	1190	H	ASP	B	30	10.577	-5.063	20.367
ATOM	1191	CA	ASP	B	30	12.609	-5.217	20.880
ATOM	1192	C	ASP	B	30	13.048	-3.886	20.335
ATOM	1193	O	ASP	B	30	12.269	-3.055	19.817
ATOM	1194	CB	ASP	B	30	12.833	-6.226	19.735
ATOM	1195	CG	ASP	B	30	12.477	-7.675	20.099
ATOM	1196	OD1	ASP	B	30	13.197	-8.272	20.908
ATOM	1197	OD2	ASP	B	30	11.494	-8.237	19.569
ATOM	1198	N	THR	B	31	14.387	-3.692	20.227
ATOM	1199	H	THR	B	31	15.018	-4.380	20.586
ATOM	1200	CA	THR	B	31	14.981	-2.530	19.614
ATOM	1201	C	THR	B	31	15.578	-2.979	18.260
ATOM	1202	O	THR	B	31	16.246	-4.020	18.123
ATOM	1203	CB	THR	B	31	16.036	-2.004	20.557
ATOM	1204	OG1	THR	B	31	15.378	-1.376	21.645
ATOM	1205	HG1	THR	B	31	16.052	-1.016	22.290
ATOM	1206	CG2	THR	B	31	16.944	-0.960	19.904
ATOM	1207	N	VAL	B	32	15.237	-2.283	17.150
ATOM	1208	H	VAL	B	32	14.703	-1.442	17.237
ATOM	1209	CA	VAL	B	32	15.626	-2.722	15.806
ATOM	1210	C	VAL	B	32	16.303	-1.566	15.132
ATOM	1211	O	VAL	B	32	15.779	-0.428	14.995
ATOM	1212	CB	VAL	B	32	14.407	-3.126	14.964
ATOM	1213	CG1	VAL	B	32	14.820	-3.703	13.596
ATOM	1214	CG2	VAL	B	32	13.556	-4.102	15.703
ATOM	1215	N	LEU	B	33	17.563	-1.756	14.720
ATOM	1216	H	LEU	B	33	17.984	-2.658	14.814
ATOM	1217	CA	LEU	B	33	18.347	-0.697	14.138
ATOM	1218	C	LEU	B	33	18.610	-1.009	12.685
ATOM	1219	O	LEU	B	33	18.685	-2.162	12.205
ATOM	1220	CB	LEU	B	33	19.679	-0.628	14.856
ATOM	1221	CG	LEU	B	33	19.698	0.363	16.031
ATOM	1222	CD1	LEU	B	33	18.425	0.321	16.891
ATOM	1223	CD2	LEU	B	33	20.929	0.179	16.889
ATOM	1224	N	GLU	B	34	18.786	0.078	11.899
ATOM	1225	H	GLU	B	34	18.619	0.991	12.271
ATOM	1226	CA	GLU	B	34	19.218	0.041	10.488
ATOM	1227	C	GLU	B	34	20.478	-0.774	10.399
ATOM	1228	O	GLU	B	34	21.374	-0.835	11.272
ATOM	1229	CB	GLU	B	34	19.536	1.460	9.996
ATOM	1230	CG	GLU	B	34	20.722	2.088	10.761

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Figure 11w

ATOM	1231	CD	GLU	B	34	21.085	3.512	10.314
ATOM	1232	OE1	GLU	B	34	20.285	4.466	10.500
ATOM	1233	OE2	GLU	B	34	22.211	3.703	9.775
ATOM	1234	N	GLU	B	35	20.673	-1.367	9.205
ATOM	1235	H	GLU	B	35	20.011	-1.227	8.468
ATOM	1236	CA	GLU	B	35	21.802	-2.205	8.930
ATOM	1237	C	GLU	B	35	23.096	-1.520	9.321
ATOM	1238	O	GLU	B	35	23.391	-0.379	8.916
ATOM	1239	CB	GLU	B	35	21.741	-2.479	7.439
ATOM	1240	CG	GLU	B	35	22.795	-3.380	6.883
ATOM	1241	CD	GLU	B	35	22.987	-4.587	7.744
ATOM	1242	OE1	GLU	B	35	21.980	-5.258	8.118
ATOM	1243	OE2	GLU	B	35	24.149	-4.860	8.048
ATOM	1244	N	MET	B	36	23.926	-2.106	10.157
ATOM	1245	H	MET	B	36	23.654	-2.953	10.613
ATOM	1246	CA	MET	B	36	25.232	-1.559	10.441
ATOM	1247	C	MET	B	36	26.146	-2.687	10.815
ATOM	1248	O	MET	B	36	25.731	-3.783	11.257
ATOM	1249	CB	MET	B	36	25.251	-0.424	11.497
ATOM	1250	CG	MET	B	36	24.626	-0.724	12.881
ATOM	1251	SD	MET	B	36	24.722	0.719	13.988
ATOM	1252	CE	MET	B	36	23.132	1.586	13.692
ATOM	1253	N	SER	B	37	27.441	-2.551	10.593
ATOM	1254	H	SER	B	37	27.783	-1.726	10.144
ATOM	1255	CA	SER	B	37	28.321	-3.608	11.011
ATOM	1256	C	SER	B	37	28.721	-3.352	12.442
ATOM	1257	O	SER	B	37	29.402	-2.369	12.788
ATOM	1258	CB	SER	B	37	29.567	-3.622	10.109
ATOM	1259	OG	SER	B	37	29.231	-3.908	8.750
ATOM	1260	HG	SER	B	37	30.057	-3.911	8.187
ATOM	1261	N	LEU	B	38	28.469	-4.295	13.366
ATOM	1262	H	LEU	B	38	27.948	-5.123	13.117
ATOM	1263	CA	LEU	B	38	29.073	-4.232	14.714
ATOM	1264	C	LEU	B	38	30.132	-5.342	14.895
ATOM	1265	O	LEU	B	38	30.070	-6.357	14.197
ATOM	1266	CB	LEU	B	38	27.986	-4.237	15.802
ATOM	1267	CG	LEU	B	38	27.005	-3.039	15.750
ATOM	1268	CD1	LEU	B	38	25.885	-3.214	16.788
ATOM	1269	CD2	LEU	B	38	27.707	-1.696	16.017
ATOM	1270	N	PRO	B	39	31.119	-5.160	15.804
ATOM	1271	CA	PRO	B	39	32.199	-6.116	16.052
ATOM	1272	C	PRO	B	39	31.767	-7.223	17.028
ATOM	1273	O	PRO	B	39	31.448	-6.942	18.185
ATOM	1274	CB	PRO	B	39	33.347	-5.276	16.625
ATOM	1275	CG	PRO	B	39	32.634	-4.148	17.370
ATOM	1276	CD	PRO	B	39	31.385	-3.916	16.523
ATOM	1277	N	GLY	B	40	31.770	-8.481	16.559
ATOM	1278	H	GLY	B	40	32.036	-8.641	15.598
ATOM	1279	CA	GLY	B	40	31.420	-9.658	17.353
ATOM	1280	C	GLY	B	40	30.679	-10.723	16.539
ATOM	1281	O	GLY	B	40	30.647	-10.671	15.308
ATOM	1282	N	LYS	B	41	30.098	-11.699	17.255
ATOM	1283	H	LYS	B	41	30.164	-11.656	18.261
ATOM	1284	CA	LYS	B	41	29.399	-12.861	16.702
ATOM	1285	C	LYS	B	41	27.971	-12.923	17.245
ATOM	1286	O	LYS	B	41	27.743	-12.700	18.436

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ATOM	1343	2HZ	LYS	B	45	14.772	-14.306	19.023
ATOM	1344	N	MET	B	46	14.240	-14.005	13.416
ATOM	1345	H	MET	B	46	13.991	-14.705	14.085
ATOM	1346	CA	MET	B	46	13.203	-13.472	12.570
ATOM	1347	C	MET	B	46	12.291	-12.623	13.425
ATOM	1348	O	MET	B	46	11.782	-13.063	14.471
ATOM	1349	CB	MET	B	46	12.383	-14.616	12.016
ATOM	1350	CG	MET	B	46	13.153	-15.586	11.187
ATOM	1351	SD	MET	B	46	12.977	-15.188	9.473
ATOM	1352	CE	MET	B	46	13.566	-16.690	8.775
ATOM	1353	N	ILE	B	47	11.933	-11.379	13.030
ATOM	1354	H	ILE	B	47	12.327	-10.991	12.196
ATOM	1355	CA	ILE	B	47	10.971	-10.568	13.797
ATOM	1356	C	ILE	B	47	9.761	-10.233	12.962
ATOM	1357	O	ILE	B	47	9.819	-10.048	11.731
ATOM	1358	CB	ILE	B	47	11.608	-9.294	14.385
ATOM	1359	CG1	ILE	B	47	12.345	-8.459	13.318
ATOM	1360	CG2	ILE	B	47	12.542	-9.638	15.494
ATOM	1361	CD1	ILE	B	47	12.789	-7.123	13.851
ATOM	1362	N	GLY	B	48	8.557	-10.136	13.558
ATOM	1363	H	GLY	B	48	8.484	-10.249	14.549
ATOM	1364	CA	GLY	B	48	7.365	-9.872	12.800
ATOM	1365	C	GLY	B	48	6.826	-8.512	13.141
ATOM	1366	O	GLY	B	48	7.136	-7.832	14.149
ATOM	1367	N	GLY	B	49	5.940	-8.027	12.306
ATOM	1368	H	GLY	B	49	5.668	-8.562	11.506
ATOM	1369	CA	GLY	B	49	5.336	-6.745	12.493
ATOM	1370	C	GLY	B	49	4.082	-6.786	11.674
ATOM	1371	O	GLY	B	49	3.561	-7.847	11.273
ATOM	1372	N	ILE	B	50	3.531	-5.634	11.315
ATOM	1373	H	ILE	B	50	4.015	-4.777	11.492
ATOM	1374	CA	ILE	B	50	2.247	-5.573	10.673
ATOM	1375	C	ILE	B	50	2.118	-6.456	9.420
ATOM	1376	O	ILE	B	50	1.175	-7.253	9.215
ATOM	1377	CB	ILE	B	50	1.982	-4.071	10.391
ATOM	1378	CG1	ILE	B	50	1.005	-3.539	11.396
ATOM	1379	CG2	ILE	B	50	1.610	-3.739	8.922
ATOM	1380	CD1	ILE	B	50	-0.391	-4.077	11.252
ATOM	1381	N	GLY	B	51	3.113	-6.410	8.519
ATOM	1382	H	GLY	B	51	3.957	-5.920	8.737
ATOM	1383	CA	GLY	B	51	2.926	-7.075	7.259
ATOM	1384	C	GLY	B	51	3.671	-8.391	7.077
ATOM	1385	O	GLY	B	51	3.716	-8.945	5.973
ATOM	1386	N	GLY	B	52	4.296	-8.982	8.116
ATOM	1387	H	GLY	B	52	4.227	-8.580	9.029
ATOM	1388	CA	GLY	B	52	5.053	-10.190	7.874
ATOM	1389	C	GLY	B	52	6.334	-10.178	8.678
ATOM	1390	O	GLY	B	52	6.519	-9.421	9.657
ATOM	1391	N	PHE	B	53	7.325	-11.015	8.343
ATOM	1392	H	PHE	B	53	7.227	-11.603	7.540
ATOM	1393	CA	PHE	B	53	8.542	-11.096	9.110
ATOM	1394	C	PHE	B	53	9.727	-10.584	8.315
ATOM	1395	O	PHE	B	53	9.780	-10.618	7.075
ATOM	1396	CB	PHE	B	53	8.804	-12.555	9.542
ATOM	1397	CG	PHE	B	53	7.850	-13.023	10.592
ATOM	1398	CD1	PHE	B	53	6.513	-13.277	10.279



Figure 11aa

ATOM	1455	CB	GLN	B	58	20.051	-11.190	17.932
ATOM	1456	CG	GLN	B	58	19.765	-10.845	19.366
ATOM	1457	CD	GLN	B	58	19.179	-12.003	20.112
ATOM	1458	OE1	GLN	B	58	19.712	-12.472	21.101
ATOM	1459	NE2	GLN	B	58	18.055	-12.476	19.623
ATOM	1460	1HE2	GLN	B	58	17.598	-13.249	20.063
ATOM	1461	2HE2	GLN	B	58	17.647	-12.066	18.807
ATOM	1462	N	TYR	B	59	22.416	-8.692	18.422
ATOM	1463	H	TYR	B	59	21.788	-7.921	18.311
ATOM	1464	CA	TYR	B	59	23.631	-8.486	19.161
ATOM	1465	C	TYR	B	59	23.244	-8.290	20.607
ATOM	1466	O	TYR	B	59	22.178	-7.728	20.927
ATOM	1467	CB	TYR	B	59	24.387	-7.241	18.653
ATOM	1468	CG	TYR	B	59	24.271	-7.075	17.149
ATOM	1469	CD1	TYR	B	59	23.045	-7.242	16.494
ATOM	1470	CD2	TYR	B	59	25.385	-6.753	16.374
ATOM	1471	CE1	TYR	B	59	22.939	-7.093	15.112
ATOM	1472	CE2	TYR	B	59	25.291	-6.603	14.995
ATOM	1473	CZ	TYR	B	59	24.068	-6.774	14.365
ATOM	1474	OH	TYR	B	59	24.018	-6.620	13.010
ATOM	1475	HH	TYR	B	59	24.926	-6.394	12.658
ATOM	1476	N	ASP	B	60	24.010	-8.785	21.596
ATOM	1477	H	ASP	B	60	24.852	-9.276	21.372
ATOM	1478	CA	ASP	B	60	23.644	-8.624	22.992
ATOM	1479	C	ASP	B	60	24.556	-7.595	23.615
ATOM	1480	O	ASP	B	60	25.654	-7.261	23.125
ATOM	1481	CB	ASP	B	60	23.789	-9.920	23.777
ATOM	1482	CG	ASP	B	60	22.803	-10.960	23.332
ATOM	1483	OD1	ASP	B	60	21.619	-10.634	23.032
ATOM	1484	OD2	ASP	B	60	23.208	-12.126	23.273
ATOM	1485	N	GLN	B	61	24.156	-7.022	24.774
ATOM	1486	H	GLN	B	61	23.252	-7.234	25.146
ATOM	1487	CA	GLN	B	61	25.011	-6.086	25.519
ATOM	1488	C	GLN	B	61	25.411	-4.866	24.746
ATOM	1489	O	GLN	B	61	26.560	-4.382	24.832
ATOM	1490	CB	GLN	B	61	26.269	-6.763	26.028
ATOM	1491	CG	GLN	B	61	26.020	-8.038	26.753
ATOM	1492	CD	GLN	B	61	25.714	-7.766	28.185
ATOM	1493	OE1	GLN	B	61	24.572	-7.455	28.548
ATOM	1494	NE2	GLN	B	61	26.744	-7.844	29.014
ATOM	1495	1HE2	GLN	B	61	26.620	-7.675	29.992
ATOM	1496	2HE2	GLN	B	61	27.654	-8.073	28.669
ATOM	1497	N	ILE	B	62	24.539	-4.257	23.933
ATOM	1498	H	ILE	B	62	23.628	-4.648	23.801
ATOM	1499	CA	ILE	B	62	24.878	-3.047	23.238
ATOM	1500	C	ILE	B	62	24.571	-1.885	24.144
ATOM	1501	O	ILE	B	62	23.515	-1.819	24.819
ATOM	1502	CB	ILE	B	62	24.097	-2.922	21.912
ATOM	1503	CG1	ILE	B	62	24.310	-4.170	21.094
ATOM	1504	CG2	ILE	B	62	24.568	-1.709	21.067
ATOM	1505	CD1	ILE	B	62	25.794	-4.479	20.878
ATOM	1506	N	LEU	B	63	25.485	-0.912	24.304
ATOM	1507	H	LEU	B	63	26.403	-1.028	23.926
ATOM	1508	CA	LEU	B	63	25.192	0.322	25.015
ATOM	1509	C	LEU	B	63	24.630	1.296	24.030
ATOM	1510	O	LEU	B	63	25.239	1.658	22.995

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ATOM	1511	CB	LEU	B	63	26.436	0.970	25.590
ATOM	1512	CG	LEU	B	63	26.186	2.358	26.226
ATOM	1513	CD1	LEU	B	63	25.486	2.261	27.576
ATOM	1514	CD2	LEU	B	63	27.468	3.162	26.382
ATOM	1515	N	ILE	B	64	23.492	1.946	24.358
ATOM	1516	H	ILE	B	64	22.958	1.643	25.148
ATOM	1517	CA	ILE	B	64	23.003	3.068	23.617
ATOM	1518	C	ILE	B	64	22.872	4.194	24.612
ATOM	1519	O	ILE	B	64	22.915	4.007	25.846
ATOM	1520	CB	ILE	B	64	21.634	2.701	22.988
ATOM	1521	CG1	ILE	B	64	21.825	1.521	22.029
ATOM	1522	CG2	ILE	B	64	20.982	3.894	22.246
ATOM	1523	CD1	ILE	B	64	20.593	1.096	21.260
ATOM	1524	N	GLU	B	65	22.803	5.460	24.172
ATOM	1525	H	GLU	B	65	23.013	5.664	23.216
ATOM	1526	CA	GLU	B	65	22.432	6.551	25.037
ATOM	1527	C	GLU	B	65	21.242	7.194	24.373
ATOM	1528	O	GLU	B	65	21.312	7.729	23.257
ATOM	1529	CB	GLU	B	65	23.497	7.615	25.131
ATOM	1530	CG	GLU	B	65	24.787	7.196	25.761
ATOM	1531	CD	GLU	B	65	25.694	8.385	26.076
ATOM	1532	OE1	GLU	B	65	25.170	9.510	26.311
ATOM	1533	OE2	GLU	B	65	26.938	8.200	26.092
ATOM	1534	N	ILE	B	66	20.078	7.240	25.035
ATOM	1535	H	ILE	B	66	20.010	6.835	25.947
ATOM	1536	CA	ILE	B	66	18.907	7.865	24.462
ATOM	1537	C	ILE	B	66	18.777	9.195	25.145
ATOM	1538	O	ILE	B	66	18.591	9.303	26.379
ATOM	1539	CB	ILE	B	66	17.713	6.995	24.790
ATOM	1540	CG1	ILE	B	66	17.916	5.583	24.335
ATOM	1541	CG2	ILE	B	66	16.405	7.544	24.177
ATOM	1542	CD1	ILE	B	66	16.888	4.677	24.884
ATOM	1543	N	CYS	B	67	18.965	10.325	24.437
ATOM	1544	H	CYS	B	67	19.201	10.268	23.467
ATOM	1545	CA	CYS	B	67	18.833	11.663	25.049
ATOM	1546	C	CYS	B	67	19.637	11.781	26.319
ATOM	1547	O	CYS	B	67	19.235	12.400	27.328
ATOM	1548	CB	CYS	B	67	17.387	12.023	25.319
ATOM	1549	SG	CYS	B	67	16.407	12.259	23.821
ATOM	1550	N	GLY	B	68	20.830	11.180	26.383
ATOM	1551	H	GLY	B	68	21.158	10.646	25.604
ATOM	1552	CA	GLY	B	68	21.654	11.288	27.558
ATOM	1553	C	GLY	B	68	21.464	10.185	28.584
ATOM	1554	O	GLY	B	68	22.174	10.128	29.606
ATOM	1555	N	HIS	B	69	20.513	9.255	28.425
ATOM	1556	H	HIS	B	69	19.924	9.282	27.618
ATOM	1557	CA	HIS	B	69	20.304	8.199	29.391
ATOM	1558	C	HIS	B	69	20.861	6.936	28.811
ATOM	1559	O	HIS	B	69	20.589	6.560	27.647
ATOM	1560	CB	HIS	B	69	18.832	7.992	29.654
ATOM	1561	CG	HIS	B	69	18.175	9.203	30.223
ATOM	1562	ND1	HIS	B	69	17.504	9.195	31.435
ATOM	1563	HD1	HIS	B	69	17.383	8.402	32.032
ATOM	1564	CD2	HIS	B	69	18.122	10.470	29.729
ATOM	1565	CE1	HIS	B	69	17.070	10.429	31.626
ATOM	1566	NE2	HIS	B	69	17.410	11.240	30.635

Figure 11<sub>cc</sub>

ATOM	1567	N	LYS	B	70	21.751	6.217	29.499
ATOM	1568	H	LYS	B	70	22.025	6.512	30.414
ATOM	1569	CA	LYS	B	70	22.326	5.020	28.945
ATOM	1570	C	LYS	B	70	21.386	3.854	29.145
ATOM	1571	O	LYS	B	70	20.627	3.725	30.120
ATOM	1572	CB	LYS	B	70	23.613	4.678	29.663
ATOM	1573	CG	LYS	B	70	24.694	5.655	29.379
ATOM	1574	CD	LYS	B	70	25.739	5.524	30.444
ATOM	1575	CE	LYS	B	70	27.048	6.090	30.011
ATOM	1576	NZ	LYS	B	70	26.948	7.548	30.000
ATOM	1577	1HZ	LYS	B	70	27.821	7.940	29.711
ATOM	1578	3HZ	LYS	B	70	26.725	7.874	30.919
ATOM	1579	2HZ	LYS	B	70	26.230	7.828	29.363
ATOM	1580	N	ALA	B	71	21.512	2.849	28.284
ATOM	1581	H	ALA	B	71	22.141	2.934	27.512
ATOM	1582	CA	ALA	B	71	20.762	1.630	28.432
ATOM	1583	C	ALA	B	71	21.629	0.576	27.805
ATOM	1584	O	ALA	B	71	22.463	0.830	26.912
ATOM	1585	CB	ALA	B	71	19.452	1.726	27.737
ATOM	1586	N	ILE	B	72	21.547	-0.681	28.237
ATOM	1587	H	ILE	B	72	20.864	-0.925	28.926
ATOM	1588	CA	ILE	B	72	22.424	-1.698	27.730
ATOM	1589	C	ILE	B	72	21.615	-2.938	27.462
ATOM	1590	O	ILE	B	72	20.909	-3.490	28.330
ATOM	1591	CB	ILE	B	72	23.524	-1.999	28.737
ATOM	1592	CG1	ILE	B	72	24.322	-0.735	29.090
ATOM	1593	CG2	ILE	B	72	24.442	-3.037	28.153
ATOM	1594	CD1	ILE	B	72	25.374	-1.012	30.163
ATOM	1595	N	GLY	B	73	21.609	-3.446	26.235
ATOM	1596	H	GLY	B	73	22.204	-3.054	25.534
ATOM	1597	CA	GLY	B	73	20.707	-4.545	26.062
ATOM	1598	C	GLY	B	73	20.828	-5.084	24.663
ATOM	1599	O	GLY	B	73	21.754	-4.831	23.863
ATOM	1600	N	THR	B	74	19.856	-5.905	24.271
ATOM	1601	H	THR	B	74	19.086	-6.088	24.882
ATOM	1602	CA	THR	B	74	19.869	-6.548	22.988
ATOM	1603	C	THR	B	74	19.363	-5.590	21.931
ATOM	1604	O	THR	B	74	18.338	-4.870	22.053
ATOM	1605	CB	THR	B	74	19.011	-7.801	23.074
ATOM	1606	OG1	THR	B	74	19.611	-8.683	24.013
ATOM	1607	HG1	THR	B	74	19.068	-9.519	24.092
ATOM	1608	CG2	THR	B	74	18.817	-8.496	21.705
ATOM	1609	N	VAL	B	75	20.028	-5.620	20.762
ATOM	1610	H	VAL	B	75	20.835	-6.203	20.666
ATOM	1611	CA	VAL	B	75	19.630	-4.837	19.611
ATOM	1612	C	VAL	B	75	19.600	-5.771	18.426
ATOM	1613	O	VAL	B	75	20.444	-6.673	18.230
ATOM	1614	CB	VAL	B	75	20.667	-3.712	19.395
ATOM	1615	CG1	VAL	B	75	20.473	-3.002	18.046
ATOM	1616	CG2	VAL	B	75	20.679	-2.708	20.567
ATOM	1617	N	LEU	B	76	18.557	-5.647	17.565
ATOM	1618	H	LEU	B	76	17.822	-5.000	17.767
ATOM	1619	CA	LEU	B	76	18.444	-6.427	16.324
ATOM	1620	C	LEU	B	76	18.736	-5.487	15.144
ATOM	1621	O	LEU	B	76	18.239	-4.343	15.040
ATOM	1622	CB	LEU	B	76	17.028	-7.021	16.158

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ATOM	1623	CG	LEU	B	76	16.427	-7.612	17.449
ATOM	1624	CD1	LEU	B	76	14.992	-8.075	17.263
ATOM	1625	CD2	LEU	B	76	17.266	-8.758	18.019
ATOM	1626	N	VAL	B	77	19.607	-5.900	14.222
ATOM	1627	H	VAL	B	77	19.985	-6.824	14.276
ATOM	1628	CA	VAL	B	77	20.027	-5.042	13.133
ATOM	1629	C	VAL	B	77	19.570	-5.662	11.842
ATOM	1630	O	VAL	B	77	19.678	-6.883	11.598
ATOM	1631	CB	VAL	B	77	21.563	-4.905	13.191
ATOM	1632	CG1	VAL	B	77	22.129	-4.202	11.944
ATOM	1633	CG2	VAL	B	77	22.030	-4.166	14.470
ATOM	1634	N	GLY	B	78	18.978	-4.915	10.943
ATOM	1635	H	GLY	B	78	18.841	-3.941	11.121
ATOM	1636	CA	GLY	B	78	18.523	-5.475	9.705
ATOM	1637	C	GLY	B	78	18.019	-4.338	8.874
ATOM	1638	O	GLY	B	78	18.130	-3.142	9.223
ATOM	1639	N	PRO	B	79	17.408	-4.596	7.722
ATOM	1640	CA	PRO	B	79	16.954	-3.535	6.834
ATOM	1641	C	PRO	B	79	15.635	-2.872	7.280
ATOM	1642	O	PRO	B	79	14.609	-2.877	6.565
ATOM	1643	CB	PRO	B	79	16.804	-4.274	5.492
ATOM	1644	CG	PRO	B	79	16.463	-5.712	5.881
ATOM	1645	CD	PRO	B	79	17.159	-5.959	7.189
ATOM	1646	N	THR	B	80	15.574	-2.247	8.458
ATOM	1647	H	THR	B	80	16.374	-2.242	9.058
ATOM	1648	CA	THR	B	80	14.364	-1.583	8.865
ATOM	1649	C	THR	B	80	14.312	-0.189	8.228
ATOM	1650	O	THR	B	80	15.349	0.471	8.001
ATOM	1651	CB	THR	B	80	14.250	-1.512	10.410
ATOM	1652	OG1	THR	B	80	13.079	-0.802	10.806
ATOM	1653	HG1	THR	B	80	13.022	-0.766	11.804
ATOM	1654	CG2	THR	B	80	15.519	-0.901	11.062
ATOM	1655	N	PRO	B	81	13.137	0.354	7.885
ATOM	1656	CA	PRO	B	81	13.036	1.747	7.379
ATOM	1657	C	PRO	B	81	13.363	2.732	8.484
ATOM	1658	O	PRO	B	81	13.791	3.880	8.250
ATOM	1659	CB	PRO	B	81	11.548	1.912	6.982
ATOM	1660	CG	PRO	B	81	10.819	0.674	7.488
ATOM	1661	CD	PRO	B	81	11.854	-0.387	7.797
ATOM	1662	N	VAL	B	82	13.197	2.368	9.772
ATOM	1663	H	VAL	B	82	12.940	1.427	9.992
ATOM	1664	CA	VAL	B	82	13.380	3.306	10.885
ATOM	1665	C	VAL	B	82	14.160	2.668	12.010
ATOM	1666	O	VAL	B	82	14.045	1.465	12.293
ATOM	1667	CB	VAL	B	82	11.996	3.695	11.431
ATOM	1668	CG1	VAL	B	82	12.055	4.961	12.269
ATOM	1669	CG2	VAL	B	82	10.958	3.857	10.318
ATOM	1670	N	ASN	B	83	14.963	3.422	12.775
ATOM	1671	H	ASN	B	83	15.147	4.370	12.516
ATOM	1672	CA	ASN	B	83	15.550	2.846	13.967
ATOM	1673	C	ASN	B	83	14.481	2.874	15.022
ATOM	1674	O	ASN	B	83	13.814	3.903	15.294
ATOM	1675	CB	ASN	B	83	16.743	3.639	14.472
ATOM	1676	CG	ASN	B	83	17.935	3.574	13.570
ATOM	1677	OD1	ASN	B	83	18.409	2.511	13.167



Figure 11ff

ATOM	1735	C	LEU	B	89	14.797	0.937	27.053
ATOM	1736	O	LEU	B	89	15.293	1.734	27.879
ATOM	1737	CB	LEU	B	89	16.421	0.232	25.236
ATOM	1738	CG	LEU	B	89	17.400	-0.754	24.567
ATOM	1739	CD1	LEU	B	89	18.215	0.002	23.573
ATOM	1740	CD2	LEU	B	89	18.352	-1.458	25.570
ATOM	1741	N	LEU	B	90	13.511	1.114	26.705
ATOM	1742	H	LEU	B	90	13.082	0.486	26.056
ATOM	1743	CA	LEU	B	90	12.698	2.221	27.257
ATOM	1744	C	LEU	B	90	12.537	2.060	28.751
ATOM	1745	O	LEU	B	90	12.575	3.033	29.533
ATOM	1746	CB	LEU	B	90	11.311	2.258	26.628
ATOM	1747	CG	LEU	B	90	11.232	2.730	25.168
ATOM	1748	CD1	LEU	B	90	9.808	2.744	24.642
ATOM	1749	CD2	LEU	B	90	11.831	4.105	24.982
ATOM	1750	N	THR	B	91	12.315	0.843	29.271
ATOM	1751	H	THR	B	91	12.218	0.055	28.663
ATOM	1752	CA	THR	B	91	12.210	0.634	30.699
ATOM	1753	C	THR	B	91	13.537	1.028	31.375
ATOM	1754	O	THR	B	91	13.575	1.525	32.518
ATOM	1755	CB	THR	B	91	11.893	-0.843	31.028
ATOM	1756	OG1	THR	B	91	12.919	-1.676	30.504
ATOM	1757	HG1	THR	B	91	12.722	-2.634	30.713
ATOM	1758	CG2	THR	B	91	10.599	-1.285	30.418
ATOM	1759	N	GLN	B	92	14.705	0.852	30.732
ATOM	1760	H	GLN	B	92	14.707	0.497	29.797
ATOM	1761	CA	GLN	B	92	15.920	1.190	31.433
ATOM	1762	C	GLN	B	92	16.088	2.660	31.633
ATOM	1763	O	GLN	B	92	16.807	3.137	32.527
ATOM	1764	CB	GLN	B	92	17.127	0.680	30.682
ATOM	1765	CG	GLN	B	92	17.076	-0.805	30.517
ATOM	1766	CD	GLN	B	92	18.336	-1.314	29.900
ATOM	1767	OE1	GLN	B	92	19.394	-0.720	30.059
ATOM	1768	NE2	GLN	B	92	18.221	-2.411	29.195
ATOM	1769	1HE2	GLN	B	92	19.022	-2.813	28.751
ATOM	1770	2HE2	GLN	B	92	17.331	-2.856	29.095
ATOM	1771	N	ILE	B	93	15.538	3.512	30.746
ATOM	1772	H	ILE	B	93	15.016	3.153	29.972
ATOM	1773	CA	ILE	B	93	15.693	4.937	30.899
ATOM	1774	C	ILE	B	93	14.522	5.549	31.698
ATOM	1775	O	ILE	B	93	14.438	6.773	31.940
ATOM	1776	CB	ILE	B	93	15.981	5.657	29.548
ATOM	1777	CG1	ILE	B	93	14.746	5.718	28.619
ATOM	1778	CG2	ILE	B	93	17.223	5.060	28.874
ATOM	1779	CD1	ILE	B	93	14.946	6.734	27.488
ATOM	1780	N	GLY	B	94	13.617	4.731	32.263
ATOM	1781	H	GLY	B	94	13.639	3.752	32.060
ATOM	1782	CA	GLY	B	94	12.594	5.224	33.170
ATOM	1783	C	GLY	B	94	11.443	5.846	32.432
ATOM	1784	O	GLY	B	94	10.766	6.803	32.878
ATOM	1785	N	CYS	B	95	11.134	5.354	31.225
ATOM	1786	H	CYS	B	95	11.603	4.538	30.888
ATOM	1787	CA	CYS	B	95	10.134	5.969	30.381
ATOM	1788	C	CYS	B	95	8.750	5.512	30.764
ATOM	1789	O	CYS	B	95	8.478	4.309	31.006
ATOM	1790	CB	CYS	B	95	10.456	5.643	28.922

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Figure 1199

ATOM	1791	SG	CYS	B	95	9.426	6.512	27.764
ATOM	1792	N	THR	B	96	7.778	6.444	30.764
ATOM	1793	H	THR	B	96	8.014	7.401	30.539
ATOM	1794	CA	THR	B	96	6.379	6.163	31.108
ATOM	1795	C	THR	B	96	5.390	6.970	30.254
ATOM	1796	O	THR	B	96	5.567	8.171	30.066
ATOM	1797	CB	THR	B	96	6.111	6.439	32.604
ATOM	1798	OG1	THR	B	96	6.341	7.794	32.938
ATOM	1799	HG1	THR	B	96	6.111	7.924	33.861
ATOM	1800	CG2	THR	B	96	6.938	5.566	33.554
ATOM	1801	N	LEU	B	97	4.302	6.321	29.809
ATOM	1802	H	LEU	B	97	4.216	5.332	29.997
ATOM	1803	CA	LEU	B	97	3.127	6.986	29.238
ATOM	1804	C	LEU	B	97	2.336	7.681	30.358
ATOM	1805	O	LEU	B	97	2.350	7.221	31.499
ATOM	1806	CB	LEU	B	97	2.226	5.958	28.532
ATOM	1807	CG	LEU	B	97	2.860	5.279	27.300
ATOM	1808	CD1	LEU	B	97	2.101	3.986	26.957
ATOM	1809	CD2	LEU	B	97	2.842	6.216	26.085
ATOM	1810	N	ASN	B	98	1.637	8.777	30.024
ATOM	1811	H	ASN	B	98	1.662	9.086	29.063
ATOM	1812	CA	ASN	B	98	0.906	9.631	30.960
ATOM	1813	C	ASN	B	98	-0.251	10.321	30.231
ATOM	1814	O	ASN	B	98	-0.032	11.303	29.522
ATOM	1815	CB	ASN	B	98	1.845	10.678	31.587
ATOM	1816	CG	ASN	B	98	2.783	10.077	32.634
ATOM	1817	OD1	ASN	B	98	3.926	9.739	32.335
ATOM	1818	ND2	ASN	B	98	2.297	9.942	33.870
ATOM	1819	2HD2	ASN	B	98	2.877	9.551	34.599
ATOM	1820	1HD2	ASN	B	98	1.351	10.229	34.074
ATOM	1821	N	LEU	B	99	-1.476	9.808	30.426
ATOM	1822	H	LEU	B	99	-1.568	9.010	31.037
ATOM	1823	CA	LEU	B	99	-2.709	10.288	29.797
ATOM	1824	C	LEU	B	99	-3.816	10.589	30.815
ATOM	1825	O	LEU	B	99	-3.630	10.272	32.011
ATOM	1826	CB	LEU	B	99	-3.146	9.340	28.657
ATOM	1827	CG	LEU	B	99	-3.714	7.932	28.941
ATOM	1828	CD1	LEU	B	99	-2.767	7.057	29.774
ATOM	1829	CD2	LEU	B	99	-5.134	7.943	29.528
ATOM	1830	OXT	LEU	B	99	-4.842	11.156	30.376
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